Dynamical correlation functions expressed in terms of many-particle *ground-state* wavefunction; the *dynamical* self-energy operator *

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We explicitly calculate the four leading-order terms of the formal asymptotic series for large $|\varepsilon|$ (where ε denotes the external energy parameter) of the single-particle Green function $G_\sigma(\varepsilon)$, $\sigma \in \{-\mathsf{s}, -\mathsf{s}+1, \dots, \mathsf{s}\}$, and the three leading-order terms of that of the self-energy operator $\Sigma_\sigma(\varepsilon)$, pertaining to systems of spin-s fermions (s = a half-integer) in d-dimensional spatial space, interacting through an arbitrary two-body potential $v(\boldsymbol{r}-\boldsymbol{r}')$. These contributions, which are expressed in terms at most of a three-body static *ground-state* correlation function, are amenable to accurate numerical calculation through employing correlated many-particle *ground-state* wavefunctions such as determined within, e.g., the quantum Monte Carlo framework. Such calculations will provide indisputably reliable information with regard to the spectral function of the single-particle excitations at high energies of correlated systems, as well as energy moments of this spectral function, and thus help to assess the reliability of theoretical approaches that are applied in studying such systems. We give especial attention to $d = 3$ and $v \equiv v_c$, the long-range Coulomb potential, for which case we explicitly calculate the *five* leading-order terms of the *regularized* large-$|\varepsilon|$ asymptotic series of $\Sigma_\sigma(\varepsilon)$. Our considerations reveal some interesting aspects which are very specific to the behaviour of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ both at small *and* large values of $\|\boldsymbol{r}-\boldsymbol{r}'\|$. In particular, we show that in these systems an inhomogeneity, even on the atomic scale, in the particle spin-polarization density gives rise to a pronounced effect, directly discernible in the inverse-photo-emission spectra; we show this effect to be absent in models with v bounded at origin and those in which $v \equiv v_c$ but Umklapp processes are neglected, unless the ground state possesses long-range magnetic order. Our analyses shed light on the importance of the non-local part of the self-energy operator and disclose that some of strictly non-local contributions to this, transform into local ones upon replacing $v \not\equiv v_c$ by v_c, implying that a local approximation to $\Sigma_\sigma(\varepsilon)$ that for $v \not\equiv v_c$ proves accurate, is necessarily less accurate for $v \equiv v_c$. These findings establish a fundamental limitation of the so-called 'dynamical mean-field' approximation to $\Sigma_\sigma(\varepsilon)$, which is *strictly* local, specifically in applications where $v \equiv v_c$. We further explicitly establish some of the shortcomings of $\Sigma_\sigma(\varepsilon)$ as calculated within the framework of the many-body perturbation theory. In this context we demonstrate the empirically well-known inadequacy of the dynamically-screened exchange self-energy operator in particular for describing the photo-emission and inverse photo-emission spectra of interacting systems at intermediate and large transfer energies and put forward a workable scheme that rids this self-energy of its fundamental defects. We present ample explicit analyses of our results in terms of *un*correlated many-body wavefunctions.

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*To the memory of my mother.

I. INTRODUCTION

A. Background

Calculation of properties of interacting many-particle systems is demanding for two reasons. Firstly, determination of the required eigenstate or ensemble of eigenstates is non-trivial and, secondly, evaluation of expectation values of observables with respect to correlated many-particle wavefunctions entails evaluation of integrals over the configuration space of the system whose dimension is proportional to the number of particles in the system. For non-interacting *many-particle* systems, both of these tasks are considerably simplified: as for the first task, eigenstates of these systems can be explicitly and directly constructed from those of a one-particle problem (as we shall see, because of the specific structure of these states, there is in fact *no* need for having these in explicit form at one's disposal), and as for the second, following the fact that the expectation value of *any* operator with respect to an uncorrelated many-body state $|\boldsymbol{\xi}\rangle$ can be expressed in terms of integrals involving an associated single-particle Slater-Fock density matrix $\varrho_{\boldsymbol{\xi};\sigma}(\boldsymbol{r},\boldsymbol{r}')$ (Appendices C and F), the dimension of the space over which explicit integration has to be carried out is determined by the nature of the operator (or observable) in question and thus does *not* scale with the number of particles in the system. This is of course also *almost* [1] the case for interacting systems; however, in contrast with the non-interacting case, where integrals over a large number of particle coordinates are fully determined by normalization, in the interacting case, these integrals need to be explicitly evaluated; owing to correlation, an integral over the configuration space, which is a *product space*, does *not* in general reduce into a product of low-dimensional integrals. This distinction between un-correlated and correlated states is explicit in the fact that in contrast with $\{\varrho_{\boldsymbol{\xi};\sigma}\}$, the single-particle density matrices pertaining to correlated states are *not* idempotent.

In view of our later considerations in this work, let us here briefly touch upon some of the crucial aspects that are involved in the calculation of the single-particle excitation energies of N-particle systems of fermions, as encoded in the single-particle Green function (GF) $G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (see § III.A). For systems with a small number of particles, the number of excited states whose energies are confined within a finite interval, is limited (here we disregard the case where such interval contains an accumulation point of the excitation spectrum), [2] so that for such systems, calculation of the single-particle excitation energies over a finite range of energies is in principle feasible. In the thermodynamic limit, where the density of the single-particle excitation energies transforms into a continuum, [3] calculation of these energies over a finite range amounts to calculation of a vast number of excited many-particle states and accordingly to that of a vast number of excited-states expectation values, which evidently *cannot* be practicable.

It is very seldom the case that an interacting many-body Hamiltonian can be exactly diagonalized so that, in general, eigenstates of interacting systems must be obtained numerically. This task is greatly simplified if the ground state (GS) and possibly a small number of lowest-lying excited states are in demand, in which cases iterative methods, notably the Lanczos method (Golub and van Loan 1983), are very effective specifically because of the fact that their application does not require storage of the entire Hamiltonian matrix (in some appropriate representation), which in general is prohibitively large. With reference to our above remarks, it is evident that for large systems, in particular those which are intended to mimic systems in the thermodynamic limit, the energies corresponding to a 'small' number of lowest-lying eigenstates do not extend over an interval of any significant width, so that for these systems the numerical method of 'exact diagonalization' is of severely limited potentiality as regards study of the excitation spectra (i.e. those corresponding to single-particle or multi-particle excitations) of interacting systems.

Insofar as GSs are concerned, the methods of quantum Monte Carlo (QMC) (for a recent review see Foulkes, *et al.* (2001)) are of considerable interest. These provide

[1] 'Almost', because here in general the single-particle density matrix does *not* suffice, but some higher-order correlation functions are required.

[2] The completeness of eigenstates of self-adjoint operators, following the Bolzano-Weierstrass theorem (Whittaker and Watson 1927, pp. 12 and 13), implies that the eigenvalues of these must possess *at least* one point of accumulation.

[3] The separation between the energy levels of a *non*-interacting system scales like L^{-2} (Landau and Lifshitz 1980, p. 14), where L stands for the macroscopic length of the system (here we neglect the possibility of occurrence of gaps in the excitation spectra brought about through the presence of some possible external potential). Interaction amongst particles complicates this picture in that each single-particle excitation energy of an interacting system (that is $\varepsilon_{s;\sigma}$ as defined in Eq. (19)) is some weighted average of a distribution of the 'non-interacting' single-particle excitation energies (that is $\{\varepsilon_{\varsigma;\sigma}^{(0)}\}$ as introduced in Eq. (56)). This aspect, together with the over-completeness of the set $\{f_{s;\sigma}(\boldsymbol{r})\}$ (see Appendix A), can in principle give rise to a large degree of degeneracy in the single-particle energy levels. These mechanisms are equally operative in finite systems or those containing finite number of particles.

both very accurate approximate GS wavefunctions for interacting systems and an effective method, based on the scheme of 'importance sampling' (for example Negele and Orland (1988, chapter 8)), for evaluating the aforementioned multi-dimensional integrals that are encountered in the calculation of expectation values. In fact, making use of a generalization of the variational principle, it is possible within the QMC formalism to construct accurate variational wavefunctions for the excited states of interacting systems; however the prospects of this approach are limited by the fact that each variational excited state is required to be orthogonal onto the lower-lying *exact* eigenstates (Peierls 1979; § 3.5 herein). Further, here, as in the framework of the 'exact-diagonalization' approach, the maximum range covered by the energies of the excited states that one may possibly be able to calculate, diminishes progressively for systems of increasing extent, so much so that, within this formalism *rigorous* calculations of the excitation spectra over a finite energy range become impracticable for systems that are intended to mimic those in the thermodynamic limit. In this connection we should like to emphasize that the difficulties associated with the transformation of the distribution of the single-particle excitation energies into continuum, in consequence of effecting the thermodynamic limit, remain even in cases where in appropriate representations the *non*-interacting single-particle energies are, in the thermodynamic limit, discrete and in general widely separated. For concreteness, consider homogeneous systems of fermions, with uniform GSs, and periodic solids. For vanishing coupling constant of interaction, in the former systems the single-particle excitations and their energies are uniquely specified in terms of the wave-vector $\boldsymbol{k}$ and spin index σ; in the latter systems, for each $(\boldsymbol{k}, \sigma)$ there is a discrete set of single-particle states, each marked in addition to $\boldsymbol{k}$ (now a *reduced* wave-vector) and σ, by an integer-valued index ℓ (band index), whose corresponding energies are in general widely separated. In these systems, an interaction of even infinitesimally weak strength brings about a *continuous* distribution of single-particle excitations whose energies envelope (not necessarily symmetrically) the well-defined and well-separated (band) energies of the corresponding non-interacting systems (see Appendix A; see also footnote 2). This phenomenon is precisely that which gives rise to the broadening of infinitely sharp peaks along the energy axis of the momentum representation of the single-particle spectral functions of non-interacting systems (here, the homogeneous systems with uniform GSs *and* periodic solids) upon switching on of the inter-particle interaction and is interpreted as corresponding to the finite lifetimes of the single-particle excitations in interacting systems (see § III.D). It follows that, for the systems just considered, even by projecting the many-body Hamiltonian on to $(N \pm 1)$-particle Hilbert spaces characterized by the (reduced) wave-vector $\boldsymbol{k}$, in general the number of $(N \pm 1)$-particle excited states whose energies (as measured with respect to the energy of the N-particle GS) cover a *finite* interval of energy, remain prohibitively large for systems that are supposed to approximate those in the thermodynamic limit.

The above considerations make evident that in general determination of the properties of the excited states of interacting systems is a demanding task, in particular when large systems with large number of particles are concerned. This aspect persists even when one's interest is narrowed to the calculation of the low-lying single-particle excitations spectra of these systems.

B. Scope of the present work

In this work we put forward an approach for the determination of the single-particle GF $G_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ and the associated self-energy (SE) $\Sigma_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ for *large* values of $|\varepsilon|$ (see later, specifically §§ II.B and III.E), formulated solely in terms of the GS expectation values of *static* operators, namely the GS number densities $n_\sigma(\boldsymbol{r})$, $\sigma \in \{-\mathsf{s}, -\mathsf{s}+1, \dots, \mathsf{s}\}$, the GS density matrices $\varrho_\sigma(\boldsymbol{r}', \boldsymbol{r})$, etc. These functions can be relatively easily calculated within the framework of the existing QMC techniques *or* that of the *local Ansatz* (Stollhoff and Fulde 1980, Stollhoff 1996, 1998) which deals with construction of variational GS wavefunctions with especial emphasis on the atomic or 'local' GS correlations. Knowledge of the asymptotic behaviour of $\Sigma_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ for large $|\varepsilon|$ enables one to calculate directly the single-particle excitation energies of interacting systems at large energies. In this paper we explicitly calculate *all* asymptotic contributions to $\Sigma_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ decaying not faster than $1/\varepsilon^2$ for $|\varepsilon| \to \infty$.

In order to illustrate the physical as well as practical relevance of the above-mentioned asymptotic contributions (see also § III.E), we point out that the leading asymptotic contribution to $\Sigma_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ for $|\varepsilon| \to \infty$ is equal to $\Sigma^{\rm HF}(\boldsymbol{r}, \boldsymbol{r}'; [\varrho_\sigma])$, the Hartree-Fock exchange SE (Farid 1999a,c), [4] as evaluated in terms of the *exact* GS single-particle density matrix ϱ_σ; $\Sigma^{\rm HF}(\boldsymbol{r}, \boldsymbol{r}'; [\varrho_\sigma])$ deviates from the Hartree plus exchange SE as determined within the framework of the (self-consistent) Hartree-Fock scheme by the fact that, in the latter, $\varrho_\sigma(\boldsymbol{r}', \boldsymbol{r})$ is replaced by its Slater-Fock counterpart $\varrho_{{\rm s};\sigma}(\boldsymbol{r}', \boldsymbol{r})$ which in strict contrast with $\varrho_\sigma(\boldsymbol{r}', \boldsymbol{r})$, is idempotent (see § III.F). Considering the fact that the significance of the asymptotic contributions to $\Sigma_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon) - \Sigma^{\rm HF}(\boldsymbol{r}, \boldsymbol{r}'; [\varrho_\sigma])$ for $|\varepsilon| \to \infty$ is controlled by the small parameter e_0/ε (where e_0 stands for an energy scale characteristic of the system under consideration; see §§ II.B and III.E),

[4] The dependence on σ of this contribution to the SE is solely through that of ϱ_σ (see § III.F.1).

while taking into account the relative accuracy of the Hartree-Fock single-particle excitation energies of specifically non-extensive interacting systems (a fact attested by the popularity of this scheme in quantum chemical applications (for example Szabo and Ostlund (1989))), it follows that the asymptotic contributions to $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ for $|\varepsilon| \to \infty$ are physically significant. This aspect of these terms should be compared with that of the terms in the perturbation series for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ as determined within the framework of the conventional many-body perturbation theory (for example Fetter and Walecka (1971)), where in contrast with e_0/ε, the strength of perturbation (or the dimensionless value of the coupling constant of the particle-particle interaction) is fixed and cannot be changed at will. [5] In fact, as we explicitly demonstrate in this work (§ IV), the leading *perturbative* contribution to $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon) - \Sigma^{\rm HF}(\boldsymbol{r},\boldsymbol{r}';[\varrho_\sigma])$, in terms of the dynamically screened interaction function $W(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (Hubbard 1957) rather than the bare one, $v(\boldsymbol{r}-\boldsymbol{r}')$, does *not* fully reproduce even the leading asymptotic contribution to $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon) - \Sigma^{\rm HF}(\boldsymbol{r},\boldsymbol{r}';[\varrho_\sigma])$ for $|\varepsilon| \to \infty$.

In addition to the above, the large-$|\varepsilon|$ asymptotic series (AS) for the *exact* $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ has further significance in that its correct reproduction to some finite order by an approximate expression for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, guarantees that the energy moments (see Eqs. (37) and (38)) of the associated approximate single-particle spectral function $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (see Eq. (39) for the definition) are to certain order identical with those of the *exact* $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (see also §§ I.C and III.B). These energy moments are of *direct* relevance to the energies of the single-particle excitations at large values of these energies. Conversely, *none* of the ε moments of $A_\sigma^{\rm Appr}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (with the exception of one which is determined by completeness, or closure; see Eq. (57)) is equal to the corresponding ε moment pertaining to the exact $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ when the *approximate* SE, to which $A_\sigma^{\rm Appr}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ corresponds, fails to reproduce, to *some* order, the terms in the large-$|\varepsilon|$ AS pertaining to the *exact* $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$. In this connection, we specifically analyse a well-known perturbative approximation to the SE operator, known as the *GW* approximation (Hedin 1965) (§ IV), and establish that its next-to-leading asymptotic term for $|\varepsilon| \to \infty$ consists solely of a *local* contribution, in contrast with the exact result which in addition consists of a *non*-local contribution. Given the fact that within the framework of the perturbation theory, the single-particle density matrix $\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$ that enters in the leading-order asymptotic contribution $\Sigma^{\rm HF}(\boldsymbol{r},\boldsymbol{r}';[\varrho_\sigma])$ to $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ is necessarily replaced by its Slater-Fock counterpart $\varrho_{{\rm s};\sigma}(\boldsymbol{r}',\boldsymbol{r})$, we observe that in practice *none* of the terms in the large-$|\varepsilon|$ AS of this *perturbative* approximation to $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ coincides with its exact counterpart. These observations are in conformity with the well-known fact that $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ as deduced from this approximate SE fails to reproduce the experimental photo-emission results (Hedin and Lundqvist 1969, Almbladh and Hedin 1983), even in simple metals (Aryasetiawan, *et al.* 1996) (see also Aryasetiawan and Gunnarsson (1995), Aryasetiawan and Karlsson (1996) and Farid (1997a, 1999a)).

We point out that, although $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ pertaining to Hamiltonians with unbounded spectra, has an unbounded support and exhibits, in the thermodynamic limit, a power-law decay for $|\varepsilon| \to \infty$, implying thus *unbounded* energy moments for $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ beyond some finite order, [6] nonetheless by considering the moments as being defined in terms of ε integrals over $(-E,E)$, the matrix elements of these with respect to some basis spanning the single-particle Hilbert space of the problem (see § III.B) have, to *any* finite order, well-defined and physically meaningful limits for $E \to \infty$. We consider this aspect in some detail and further expose an interplay between the *over-completeness* (Appendix A) of the set of Lehmann (1954) amplitudes (see Eq. (18)) associated with the single-particle excitations in interacting systems and the nature of the distribution of the energies of these excitations (see Eq. (19)) along the energy axis (see §§ III.B and III.D).

Some elements of the formalism introduced in this work have been presented in (Farid 1999a), in the context of exposing the significance to the framework of many-body perturbation theory of a mean-field theory that is capable of reproducing the GS number densities $n_\sigma(\boldsymbol{r})$, $\sigma \in \{-\mathsf{s}, -\mathsf{s}+1, \dots, \mathsf{s}\}$, pertaining to fully interacting systems. [7] In (Farid 1999a) we have merely considered

[5] Since the *exact* ϱ_σ *cannot* be expressed in terms of a finite-order perturbation series, it follows that already calculation of the *exact* $\Sigma^{\rm HF}(\boldsymbol{r},\boldsymbol{r}';[\varrho_\sigma])$ amounts to a prohibitive many-body problem.

[6] For uniform and isotropic systems, to leading order in the AS, this function decays like $1/|\varepsilon|^3$ (see § III.I.2). Consequently, for these systems the integral of $\varepsilon^{m-1} A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ over $(-E,E)$ is unbounded for $m \geq 3$ when $E \to \infty$. For definiteness, by the 'order' of an ε moment of $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, we refer to $(m-1)$ in the above expression.

[7] As will become apparent later in this work, the contributions to the AS of $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ for $|\varepsilon| \to \infty$ overwhelmingly involve $n_\sigma(\boldsymbol{r})$ and $\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$, the latter reducing to $n_\sigma(\boldsymbol{r})$ as $\boldsymbol{r}' \to \boldsymbol{r}$. Some of the arguments by Farid (1999a) are centred around the fact that a many-body perturbation theory based on a 'non-interacting' Hamiltonian $\widehat{H}_0$ whose GS number densities $n_\sigma(\boldsymbol{r})$, $\forall\sigma$, are identical with those pertaining to the GS of $\widehat{H}$, has the evident advantage of *exactly* reproducing (already in the zeroth order of perturbation theory) the pertinent contributions to the AS of $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ for $|\varepsilon| \to \infty$. For a detailed discussion of this subject see (Farid 1999b).

the leading term in the AS of the *exact* [8] $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, for $|\varepsilon|\to\infty$, and paid *no* attention whatever to the possible consequences of the specific features of the Coulomb potential $v_c(\boldsymbol{r}-\boldsymbol{r}')$, namely its long range for $\|\boldsymbol{r}-\boldsymbol{r}'\|\to\infty$ and its divergence for $\|\boldsymbol{r}-\boldsymbol{r}'\|\to 0$, to the behaviour of terms in this series. As we discuss in this work, these aspects of v_c are of significant influence on the behaviour of the SE *operator* $\Sigma_\sigma(\varepsilon)$ at large values of $|\varepsilon|$, both in the coordinate and in the momentum representation. In this connection it is appropriate to mention that, owing to the divergence of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ for $\|\boldsymbol{r}-\boldsymbol{r}'\|\to 0$, the nature of the AS for $\Sigma_\sigma(\varepsilon)$ is dependent upon the choice of representation; that is, depending on this, the contributions to the *complete* AS need be combined differently in order to determine the appropriate terms in a *finite*-order AS concerning $|\varepsilon|\to\infty$. In this paper, we primarily consider $\Sigma_\sigma(\varepsilon)$ in the coordinate representation; however, owing to the physical significance of $\Sigma_\sigma(\varepsilon)$ in the momentum representation, we in addition present many of the relevant expressions in this representation. We should emphasize that v_c in $d=3$ is *not* exceptional for its specific consequences to the behaviour of $\Sigma_\sigma(\varepsilon)$ at large $|\varepsilon|$, as one can conceive of other two-body potentials, and in spatial dimensions not necessarily equal to 3, for which the contributions to the AS for $\Sigma_\sigma(\varepsilon)$ at large $|\varepsilon|$ are dissimilar to those corresponding to bounded and short-range interaction potentials. The distinctive aspect of v_c in $d=3$ in the context of our present work is that, up to a multiplicative constant, it is the inverse of the single-particle kinetic-energy operator and this aspect directly results in some undefined contributions upon substitution of v_c for v in the expression for the coefficient of the $1/\varepsilon^2$ term in the formal large-$|\varepsilon|$ AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (see Eq. (72)). Since $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ is a well-defined function, any fundamentally unbounded contribution in its large-$|\varepsilon|$ AS *must* be compensated by equally fundamentally unbounded contributions in infinite number of subsequent terms in this series (see § II.B); appropriate summations over these contributions result in well-defined functions that involve transcendental functions of ε, such as $(-z/\varepsilon_0)^{1/2}/z^2$ and $\ln(-z/\varepsilon_0)/z^2$ where $z=\varepsilon\pm i\eta$, complementing the formal large-$|\varepsilon|$ AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ in terms of the asymptotic sequence $\{1,1/\varepsilon,1/\varepsilon^2,\dots\}$. Here ε_0 denotes an arbitrary positive energy so that $\varepsilon/\varepsilon_0$ is dimensionless.

As mentioned above, the large-$|\varepsilon|$ AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ with which we deal in this work, is in terms of *exact GS* correlation functions. Denoting the coefficient of $1/\varepsilon^m$ in this formal series by $\Sigma_{\sigma;\infty_m}$ (see Eq. (72)), we observe that $\Sigma_{\sigma;\infty_m}$ involves various $(m+1)$th-order combinations [9] of the single-particle kinetic-energy operator τ (see Eq. (3)), the scalar external potential u and the *bare* particle-particle interaction function v. These aspects unequivocally establish that the *exact* $\Sigma_{\sigma;\infty_m}$ would be identically reproduced by choosing as the starting point of the calculations, the *complete* $(m+1)$th-order perturbation series expansion of the SE operator, that is the series *up to and including* the $(m+1)$th-order contributions, in terms of the *bare* particle-particle interaction function and the *skeleton* SE diagrams (for the definition see Luttinger and Ward (1960)) which are determined in terms of the *exact* single-particle GF pertaining to the *interacting* system. In fact (see in particular Eq. (121) and the associated text), the *complete* AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ corresponding to $|\varepsilon|\to\infty$ is entirely equivalent with the *complete* many-body perturbation series concerning the *exact* $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ for *arbitrary* ε; the two series merely deviate by the fact that, whereas, in the perturbation series, contributions to $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ are arranged in accordance with the increasing powers of the coupling constant of v, in the AS of this function corresponding to $|\varepsilon|\to\infty$, the contributions are arranged in accordance with the increasing powers of $1/\varepsilon$. As we have indicated earlier in this Introduction (§ I.A), the latter arrangement is superior to the former for sufficiently large values of $|\varepsilon|$ (see specifically § III.E).

Similar to perturbation series where unbounded contributions are regularized through performing partial summations over *infinite* number of pertinent unbounded contributions corresponding to higher-order terms in the perturbation series, here also unbounded terms in the expressions for the coefficient functions pertaining to the asymptotic sequence $\{1,1/\varepsilon,1/\varepsilon^2,\dots\}$ are regularized through infinite summations over pertinent unbounded terms that occur in the higher-order terms as arranged in accordance with the powers of $1/\varepsilon$. For $v\equiv v_c$ and $d=3$, $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ is unbounded and, performing the latter infinite partial summations, we deduce that in this case, in a finite-order large-$|\varepsilon|$ AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, $\Sigma^{\rm HF}(\boldsymbol{r},\boldsymbol{r}';[\varrho_\sigma])+\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')/\varepsilon$ is followed by contributions that decay like $1/|\varepsilon|^{3/2}$, $\ln(|\varepsilon/\varepsilon_0|)/\varepsilon^2$, $1/\varepsilon^2$, ... rather than merely $1/\varepsilon^2$, ..., as would be expected from the *formal* structure of the AS for the SE corresponding

[8] In fact, the considerations in (Farid 1999a) are confined to systems of spin-less fermions or those of spin-1/2 fermions which are fully spin compensated.

[9] As we shall see in § III.C, from the Dyson equation it directly follows (see, e.g., footnote 38 below) that $\{\Sigma_{\sigma;\infty_p}\|p=0,1,\dots,m\}$ is the complete set necessary for the evaluation of $G_{\sigma;\infty_{m+2}}$; conversely, determination of $\Sigma_{\sigma;\infty_m}$ is dependent upon the knowledge of $\{G_{\sigma;\infty_p}\|p=0,1,\dots,m+2\}$. Through Eq. (34) below we observe that $G_{\sigma;\infty_{m+2}}$ involves $\widehat{L}^{m+1}$ which implies $m+1$ *nested* commutations with $\widehat{H}$. This underlies our above statement, "$(m+1)$th-order combinations of ...". See § II.B, the paragraph beginning with "Second, considering for the moment ...".

to an unspecified v (see Eq. (72)). In addition, we obtain that $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ involves a contribution proportional to $v^3(\boldsymbol{r}-\boldsymbol{r}')$ which, although well defined, is *not* integrable (in the sense of Riemann) in the case where $v \equiv v_c$ in $d=3$, thus demonstrating the momentum representation of $\Sigma_{\sigma;\infty_2}$ to be ill defined. This problem is removed through a further summation over an infinite number of similarly non-integrable contributions corresponding to $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ with $m>2$, giving rise to an additional singular contribution of the form $\ln(|\varepsilon/\varepsilon_0|)/\varepsilon^2$ to the AS of the momentum representation of $\Sigma_\sigma(\varepsilon)$ for $|\varepsilon|\to\infty$.

To summarize, we observe that in the cases corresponding to $v\equiv v_c$ in $d=3$, the AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, $|\varepsilon|\to\infty$, acquires *singular* contributions, corresponding to the transcendental functions $\ln(-z/\varepsilon_0)$ and $(-z/\varepsilon_0)^{1/2}$; the latter function has its origin in the particular behaviour of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ for $\|\boldsymbol{r}-\boldsymbol{r}'\|\to 0$ and its appearance in the AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ depends on the number density corresponding to particles of spin index σ is in *local* imbalance with the *total* number density of particles whose spin indices are different from σ (see Eqs. (213) and (G15)). Here, z denotes a *complex*-valued energy (see § II.B).

Although our considerations in this work are *not* in the main concerned with the behaviour of $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ for $\varepsilon\approx\varepsilon_F$, [10] with ε_F the Fermi energy (we assume for the moment metallic GSs), our above findings with regard to the existence of singular contributions corresponding to $(-z/\varepsilon_0)^{1/2}$ and $\ln(-z/\varepsilon_0)$ in the large-$|z|$ AS for $\widetilde{\Sigma}_\sigma(z)$ can be of significance for the nature of the terms to be expected in the AS for $\widetilde{\Sigma}_\sigma(z)$ corresponding to $|z-\varepsilon_F|\to 0$. [11] To clarify this statement, we first mention that $\widetilde{\Sigma}_\sigma(z)$ is analytic over the entire complex z plane with the exception of the real axis (Luttinger 1961, Farid 1999a). Consequently, the branch cuts corresponding to the branch points at the point of infinity, associated with $(-z/\varepsilon_0)^{1/2}$, $\ln(-z/\varepsilon_0)$, etc., must be connected with further singular contributions to $\widetilde{\Sigma}_\sigma(z)$ in the *finite* part of the complex energy plane, of the form $(z-\varepsilon_1)^{1/2}$, $\ln(z-\varepsilon_2)$, etc., respectively, where ε_1, ε_2, etc., are *real* and *finite*. By making the *assumption* that $\varepsilon_1=\varepsilon_2=\ldots=\varepsilon_F$, the nature of the singular functions in the small-$|z-\varepsilon_F|$ AS of $\widetilde{\Sigma}_\sigma(z)$ are directly deduced from those in the large-$|z|$ AS of this function. Thus, the results presented above would imply that, under the conditions where $(-z/\varepsilon_0)^{1/2}/z^2$ appears in the large-$|z|$ AS of $\widetilde{\Sigma}_\sigma(z)$, one should expect appearance of $(z-\varepsilon_F)^{3/2}$ in the small-$|z-\varepsilon_F|$ AS of $\widetilde{\Sigma}_\sigma(z)$. Although a contribution of this form does *not* imply breakdown of the Fermi-liquid picture for the corresponding metallic state (Farid 1999c), it nonetheless amounts to a considerable deviation from the behaviour of $\widetilde{\Sigma}_\sigma(z)$ corresponding to *conventional* Fermi liquids in $d=3$. The above assumption *cannot* in general be true; [12] however, the fact remains that branch points of $\widetilde{\Sigma}_\sigma(z)$ at the point of infinity of the complex z plane *must necessarily* have their counterparts at finite values of energies along the real ε axis. From this perspective, it is *not* excluded that breakdown of Fermi-liquid metallic states in spatial dimensions d greater than one, specifically in $d=2$, can be a consequence of the coincidence of one of the above-indicated energies $\{\varepsilon_j\}$ with ε_F. Accordingly, while attempting to establish the behaviour of $\widetilde{\Sigma}_\sigma(z)$ for $|z-\varepsilon_F|\to 0$, one may consider also to investigate the asymptotic behaviour of $\widetilde{\Sigma}_\sigma(z)$ for $|z|\to\infty$ as one of the preparatory steps.

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[10] We only very briefly touch upon $\varepsilon\approx\varepsilon_F$ in Appendix A.

[11] In this paper we denote the analytic continuation of $f(\varepsilon)$, a function of the external energy parameter ε, into the physical Riemann sheet of the z plane, that is the complex energy plane, by $\widetilde{f}(z)$ (for details, see Farid (1999a,c)). See, for instance, Eqs. (protect17) and (24) below.

[12] This assumption is, however, easily shown to be true in the case of *conventional* Fermi liquids in $d=3$ in non-magnetic GSs. Nonetheless, our observations in § IV where we investigate the large-$|z|$ AS for $\widetilde{\Sigma}_\sigma^{(1)}(z)$, the first-order contribution to $\widetilde{\Sigma}_\sigma(z)$ according to the perturbation theory in terms of the dynamically screened particle-particle interaction function $W(\varepsilon)$ and the interacting GF, imply that this assumption *cannot* be universally valid (see § V). In § IV we deduce that, *independent* of the magnetic state of the GS, in the case of $v\equiv v_c$ and $d=3$ there is a contribution proportional to $(-z/\varepsilon_0)^{1/2}/z^2$ to the large-$|z|$ AS of $\widetilde{\Sigma}_\sigma^{(1)}(z)$ which survives substitution of G_σ by its non-interacting counterpart $G_{0;\sigma}$, and of W by its random-phase approximation as determined in terms of $G_{0;\sigma}$. Yet, in spite of these, there is *no* evidence that, according to these widely used approximations, $\widetilde{\Sigma}_\sigma^{(1)}(z)$ would involve a term proportional to $(z-\varepsilon_F)^{3/2}$ in its AS for $|z-\varepsilon_F|\to 0$. Further, one can show (B. Farid, 2001, unpublished) that for a system of Coulomb-interacting fermions confined to a plane (i.e. for $d=2$), the leading, z-independent, term in the large-$|z|$ AS of $\widetilde{\Sigma}_\sigma^{(1)}(z)$ is followed by a term proportional to $(-z/\varepsilon_0)^{1/2}/z$. The appearance of $(z-\varepsilon_0)^{1/2}$ in the small-$|z-\varepsilon_F|$ AS for $\widetilde{\Sigma}_\sigma^{(1)}(z)$ would not only imply a severe breakdown of the Fermi-liquid metallic state in $d=2$, but also that the value of the corresponding anomalous exponent would far exceed that of its counterpart pertaining to the *one*-dimensional Luttinger (1963) model (Mattis and Lieb 1965) (for a review see Voit (1994)). In spite of these arguments, it is possible that, from among many branch points at the point of infinity, *some* of the associated points in $\{\varepsilon_j\|j=1,2,\ldots\}$ may coincide with ε_F (contrast with the extreme and unlikely proposition that $\varepsilon_1=\varepsilon_2=\ldots=\varepsilon_F$).

C. Narrow-band systems; a brief survey

Electronic systems with transition, rare-earth or actinide atoms, involving localized and open-shell d, $4f$ and $5f$ electrons respectively, manifest some of the most dramatic consequences of the electron-electron interaction (Fulde 1991, chapters 11, 12 and 13). The strength of correlation in these systems is almost invariably quantified in terms of the value for the *intra*-atomic energy U (I and C in the earlier literature) in relation to the width W of the tight-binding band associated with the overlap matrix element of an appropriate mean-field Hamiltonian with respect to the atomic (or Wannier) orbitals centred at the indicated atoms in neighbouring positions. Strong correlation in these systems is thus signified through the corresponding 'large' values of the dimensionless constant U/W. Such a characterization has its parallel in uniform and isotropic systems (see § III.E), with the dimensionless parameter r_s (see Eq. (94)) playing the role of U/W where to leading order and up to a multiplicative constant of the order unity (≈ -2.4), r_s is equal to the ratio of the GS expectation value of the interaction-energy operator $\widehat{V}$ (see Eq. (2)) to that of the kinetic-energy operator $\widehat{T}$, [13] establishing a direct correspondence between large values of r_s and strong correlation. Clearly, however, similar values of U/W and r_s do *not* signify comparable physical consequences. Thus, whereas at the half-filling of the one-band Hubbard model in $d = 3$ (corresponding to one electron per orbital), $U/W \approx 1.15$ is the condition for the occurrence of metal-to-insulator transition (Hubbard 1964), not until $r_s \approx 10^2$ is this transition expected in uniform-electron systems (see Ceperley and Alder (1980), and Herman and March (1984) for a detailed analysis of the data by the former authors; for a more recent study see Ortiz, *et al.* (1999)).

The low-energy physics of strongly correlated systems in which the *intra-atomic* electron-electron interaction plays a prominent role is generally described by means of the Hubbard Hamiltonian (Anderson 1959, Ruijgrok 1962, Gutzwiller 1963, Izuyama, *et al.* 1963, Hubbard 1963, Kanamori 1963) [14] in which the number of orbitals per lattice cite can be as few as one, corresponding to the 'one-band' Hubbard model. Such or comparable restrictions on the number of orbitals per cite implies that in contrast with the single-particle excitation spectrum pertaining to Hamiltonian $\widehat{H}$ in Eq. (1), that pertaining to the Hubbard Hamiltonian (or any other Hamiltonian deduced from it) is *bounded*. Consequently, $\widetilde{G}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$ and $\widetilde{\Sigma}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$ pertaining to this model [15] possess Laurent series expansions (see § II.B) for $|z|$ larger than some finite value which depends on the parameters of the Hamiltonian and d. Viewing these series as AS (see § II.B), we observe that, in dealing with the Hubbard Hamiltonian, the complications associated with the large-$|z|$ AS expansions of $\widetilde{G}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$ and $\widetilde{\Sigma}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$ pertaining to the general Hamiltonian $\widehat{H}$ in Eq. (1) do *not* arise. In other words, in the case of the Hubbard Hamiltonian, the status of E as introduced in Eq. (38) below is raised to that of a natural finite cut-off energy. Correspondingly, the energy moments integrals of the single-particle spectral function of this Hamiltonian (see Eqs. (37) and (38)) exist to any *finite* order (see § I.B). With this property at hand, the problem concerning specification of the single-particle spectral function $A_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ (see Eqs. (39) and (282)) in terms of its ε-moments integrals is reduced to the classical "problem of moments" due to Tchebycheff (i.e. Chebyshev), Markoff (i.e. Markov), Stieltjes and others (for example Shohat and Tamarkin (1943)). To clarify this statement, we note that the ε integrals in our work are Riemann integrals, specified by the Riemann measure $\mathrm{d}\varepsilon$, as opposed to Stieltjes integrals (Kreyszig 1978, pp. 225-227) [16] specified by the measure $\mathrm{d}\xi(\varepsilon)$, where $\xi(\varepsilon)$ stands for a function of bounded variation over the relevant range of ε so that, unless the single-particle spectral function $A_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ is one with exponentially decaying 'tails' or with bounded support (such as is the case with the conventional Hubbard Hamiltonian), with the exception of a small number of low-order ones, the ε moments of $A_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ pertaining to macroscopic systems do *not* exist. [17]

According to Kubo and Tomita (1954), *"the moment method"*, considered by the authors as *"the most common and basic method"* used thus far *"for the discussions of the line shapes of magnetic resonance absorption"*, was first employed in physics by Broer (1943), van Vleck (1948) and Pryce and Stevens (1951). To our knowledge, the application of the moments method in the form most akin to that discussed in § III.B of the present work is due

[13] Measuring energy in Rydberg (see Eq. (102) below) and considering $v \equiv v_c$ in $d = 3$, according to Gell-Mann and Brueckner (1957) (see also Pines and Nozières (1966)) for the total energy per particle $E_{N;0}/N$ of the paramagnetic GS of a uniform and isotropic electron system we have $E_{N;0}/N = 2.21/r_s^2 - 0.916/r_s + 0.062\ln(r_s) - 0.096 + \ldots$, from which it is seen that the ratio of the second term (i.e. the *bare* exchange energy) to the first one (i.e. the *bare* kinetic energy) is indeed proportional to r_s. See text following Eq. (101) below.

[14] For a compilation of some of the relevant papers see Montorsi (1992).

[15] Here $\boldsymbol{r}$ and $\boldsymbol{r}'$ are vectors of a discrete set which thus may be denoted by $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ respectively.

[16] For excellent treatments of the theory of Stieltjes integrals see Titchmarsh (1939) and Hobson (1927).

[17] See § III.I.2 and recall that, in general, $A_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ decays algebraically for $|\varepsilon| \to \infty$, as opposed to exponentially.

to Harris and Lange (1967) and Kalashnikov and Fradkin (1969,1973). It also significantly features in the considerations by Nagaoka (1965,1966) and Brinkman and Rice (1970a). [18] In a series of articles by Nolting (1972, 1977, 1978), Nolting and Oleś (1979,1980, 1981,1987), Nolting and Borgieł (1989), Eskes and Oleś (1994) and Eskes, *et al.* (1994), the method has been extensively applied in conjunction with a two-pole *Ansatz* for the single-particle spectral function as well as some appropriate auxiliary correlation functions (required for the purpose of achieving self-consistency in the pertinent calculations) pertaining to the Hubbard Hamiltonian. The significance of correctly reproducing the ε moments of the single-particle spectral function has been further accounted for in the construction of an approximate expression for the SE (Kajueter and Kotliar 1996) pertaining to the Hubbard Hamiltonian in $d = \infty$ (Metzner and Vollhardt 1989, Vollhardt 1993) [19] which is equivalent with the single-impurity Anderson (1961) model for the hybridized state of a single magnetic impurity and conduction electrons (Ohkawa 1991, Georges and Kotliar 1992).

The method of moments and the associated continued fraction expansions (for example, Gordon 1968) of the (single-particle) spectra of interacting systems *within mean-field approximation frameworks* have been subjects of considerable interest in the past (see Haydock 1980). In the same way that application of the moments method in the case of interacting systems (see above) offers a way out of diagonalizing an interacting Hamiltonian (albeit in exchange for certain inaccuracies), it provides an alternative to bypassing exact diagonalization of mean-field Hamiltonians. Technically, however, particle-particle interaction renders calculation of the moments considerably difficult as it prevents these from being expressed in terms of products of matrices. Our considerations in the subsequent Sections of this paper clearly expose the complexity of the required calculations; these also show the prohibitive nature of the task of regularizing various contributions to the explicit expressions for the moments integrals in the cases where the interaction potential v is not short range and bounded at zero separation of particles.

[18] For completeness, we also refer to work by Gordon (1968) which deals with the calculation of the thermodynamic properties of systems through employing the high-temperature expansion of the canonical partition function, which he formulates as a classical "problem of moments".

[19] In order to obtain a meaningful Hamiltonian for $d \to \infty$, the hopping term in the conventional Hubbard Hamiltonian is divided by $\sqrt{2d}$ prior to taking the limit $d \to \infty$ (see Metzner and Vollhardt 1989).

D. The organization of the work

In § II.A we introduce the Hamiltonian on which our general considerations in this paper are based. In order to maintain flexibility, unless we indicate otherwise the dimension of the spatial space to which the system is confined is d which is an *integer*, however under specific circumstances can be made into a real or complex quantity (Wilson 1973). [20] Similarly, we leave the spin s, corresponding to spin multiplicity $2\mathsf{s}+1$, of the fermions unspecified. [21] As our work is mainly directed towards determination of the behaviour of the single-particle GF $G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ and the SE $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ at large values of $|\varepsilon|$, in § II.B we present a detailed exposition of some specific aspects of the theory of AS of functions of complex variable z for in particular large values of $|z|$. For two reasons we have considered inclusion of this exposition to be necessary: firstly, the available texts dealing with the theory of AS are *not* sufficiently explicit in regard to the issues of primary relevance to our specific considerations in the present work; [22] secondly, the main objects of our considerations are the Green and SE *operators*, $G_\sigma(\varepsilon)$ and $\Sigma_\sigma(\varepsilon)$ respectively, of which the above *functions* are coordinate representations; it turns out that, in particular for systems of particles interacting through the Coulomb potential, these operators do *not* admit of universal and meaningful *finite-order* AS; rather such finite-order series crucially depend on the choice of the representation of these operators. In § II.B we give our full attention to this aspect, specifying the criteria for finite-order AS to be meaningful in the coordinate representation, and present the details concerning the unbounded contributions in the latter series as well as the principles underlying their regularization.

In § III we pursue the primary objective of the present work, namely determination of the general forms and explicit expressions for the terms in the formal AS corresponding to $G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ and $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ for $|\varepsilon| \to \infty$. We consider both the general case and the specific case concerning systems of fermions in $d = 3$, interacting through

[20] For a comprehensive review of the Wilson-Fisher (Wilson 1973, Wilson and Fisher 1972) theory of dimensional continuation see (Collins 1984, Chapter 4). For some specific details see (Farid 2000b). The process of dimensional continuation in the style of Metzner and Vollhardt (1989) for the purpose of evaluating the limit $d \to \infty$, requires some appropriate adjustments to the Hamiltonian of the system, so that it *cannot* be identified with the Wilson-Fisher process.

[21] Again, here we have in mind the possibility of employing such strategy as that of $1/\mathsf{s}$ expansion (see Auerbach 1993) at some future occasion.

[22] We have, however, greatly benefited from specifically the text by Dingle (1973) on the subject matter.

the Coulomb potential v_c. We present the pertinent expressions in fully regularized form, amenable to direct numerical calculation; in Appendices we present the details underlying regularization of all unbounded contributions encountered in our work. In this Section we also consider some details concerning determination of the single-particle excitation energies in interacting systems, in particular in the regime of high excitation energies where our large-$|\varepsilon|$ asymptotic results for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ can be safely and fruitfully employed. We devote the concluding parts of § III to a detailed consideration of a finite-order AS for $\mathrm{Im}\big[\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)\big]$ as $|\varepsilon|\to\infty$. Among others, these considerations clearly expose the ambiguities that can arise (and *do* arise in the case of Coulomb interacting particles) as a result of exchanging the orders of infinite sums and integrals in the process of deducing finite-order AS for $\mathrm{Im}\big[\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)\big]$ corresponding to $|\varepsilon|\to\infty$.

In § IV we deal with the SE operator as determined within the framework of the first-order perturbation theory in terms of the dynamically screened interaction function $W(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, as opposed to the bare interaction function $v(\boldsymbol{r}-\boldsymbol{r}')$. In our general considerations we assume that the perturbation series is in terms of the *exact* single-particle GF and the *exact* screened interaction function. From the corresponding results we readily deduce those specific to the case in which the single-particle GF is identified with that pertaining to a mean-field Hamiltonian. We further explicitly demonstrate the significant deviation of the second leading term in the large-$|\varepsilon|$ AS of the mentioned first-order result for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ in comparison with the corresponding exact result, as deduced and presented in § III, and put forward a practicable formalism that corrects for this and other similar deviations.

We conclude the main body of this work in § V by a summary and some remarks. In a relatively large number of Appendices (see Contents) we provide the details that either underly or are supplementary to our considerations in the main body of the paper. To facilitate use of this paper, in addition to the Contents, we provide two lists containing specifications of some of the frequently used symbols and abbreviations in this paper. Throughout this work we assume the value of the absolute temperature to be zero and the GS of the systems dealt with to be non-degenerate and *normal* (as opposed to superfluid, for instance).

II. PRELIMINARIES

A. The system and its Hamiltonian

In this work we deal with the following Hamiltonian

$$\widehat{H} = \widehat{T} + \widehat{U} + \widehat{V}, \tag{1}$$

in which [23]

$$\begin{aligned}
\widehat{T} &:= \sum_\sigma \int \mathrm{d}^d r\; \hat{\psi}_\sigma^\dagger(\boldsymbol{r})\, \tau(\boldsymbol{r})\, \hat{\psi}_\sigma(\boldsymbol{r}), \\
\widehat{U} &:= \sum_\sigma \int \mathrm{d}^d r\; \hat{\psi}_\sigma^\dagger(\boldsymbol{r})\, u(\boldsymbol{r})\, \hat{\psi}_\sigma(\boldsymbol{r}), \\
\widehat{V} &:= \frac{1}{2}\sum_{\sigma,\sigma'} \int \mathrm{d}^d r \mathrm{d}^d r'\; \hat{\psi}_\sigma^\dagger(\boldsymbol{r}) \hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r}') \\
&\qquad\qquad \times v(\boldsymbol{r}-\boldsymbol{r}')\, \hat{\psi}_{\sigma'}(\boldsymbol{r}') \hat{\psi}_\sigma(\boldsymbol{r})
\end{aligned} \tag{2}$$

are the second-quantization representations of the kinetic-energy due to the single-particle kinetic-energy operator

$$\tau(\boldsymbol{r}) := \frac{-\hbar^2}{2m_e}\, \nabla_{\boldsymbol{r}}^2, \tag{3}$$

potential energy due to the *local* electrostatic external potential $u(\boldsymbol{r})$ (e.g. ionic potential) and the particle-particle interaction energy, respectively. In Eq. (3), m_e denotes the mass of particles (e.g. electrons) and the subscript $\boldsymbol{r}$ in $\nabla_{\boldsymbol{r}}^2$ makes explicit that it operates on functions of $\boldsymbol{r}$. In what follows we leave the dimension of the spatial space, d, unspecified. Further, in our general considerations we do not specify the two-body potential v; however, at regular intervals explicitly consider the case where v is the long-range Coulomb potential in $d = 3$, which we denote by v_c. Thus, whereas, in the following, v is general and therefore may be identified with v_c, v_c is specific and, unless explicitly indicated otherwise, strictly denotes the Coulomb potential in $d = 3$. Further, unless we state to the contrary, in this paper, systems of fermions interacting through v_c are implicitly assumed to be *macroscopic*. Although our formalism is equally applicable to finite systems, independent of whether $v \equiv v_c$ or $v \not\equiv v_c$, some details of our considerations are redundant in regard to these systems.

For an appropriate treatment of the case corresponding to *macroscopic* systems of particles interacting through the Coulomb potential [24]

$$v_c(\boldsymbol{r}-\boldsymbol{r}') \equiv \frac{e^2}{4\pi\epsilon_0} \frac{1}{\|\boldsymbol{r}-\boldsymbol{r}'\|}, \tag{4}$$

with e^2 the electron charge $-e$ squared and ϵ_0 the vacuum permittivity, equal to $8.854\ldots \times 10^{-12}$ F m^{-1}, we need to supplement $\widehat{H}$ in Eq. (1) by $\widehat{H}_\kappa$, where

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[23] Here the spatial integrals are over a d-dimensional space of volume Ω. For macroscopic systems in d spatial dimensions, we consider $\Omega = L^d$, where L stands for the macroscopic length of the side of the d-dimensional hyper-cubic box into which the system is confined.

[24] Since we define v_c (see Eq. (4)) in terms of $(-e)^2$, it has the dimension *energy* and therefore is *not* a *potential* in the strict sense of the word.

$$\widehat{H}_{\kappa} := -\,\varpi_{\kappa} \widehat{N}, \quad \varpi_{\kappa} := \frac{e^2 n_0}{2\epsilon_0 \kappa^2}, \tag{5}$$

and take the limit $\kappa \downarrow 0$ at the final stage of calculations. In Eq. (5) $\widehat{N}$ stands for the *total* number operator,

$$\widehat{N} \equiv \sum_{\sigma} \widehat{N}_{\sigma}, \tag{6}$$

with

$$\widehat{N}_{\sigma} := \int \mathrm{d}^d r \; \hat{\psi}_{\sigma}^{\dagger}(\boldsymbol{r}) \hat{\psi}_{\sigma}(\boldsymbol{r}), \quad \sigma \in \{-\mathsf{s}, -\mathsf{s}+1, \dots, \mathsf{s}\}, \tag{7}$$

the *partial* number operators, which mutually commute, i.e.

$$\big[\widehat{N}_{\sigma}, \widehat{N}_{\sigma'}\big]_{-} = 0, \quad \forall\, \sigma, \sigma'. \tag{8}$$

Further, in Eq. (5)

$$n_0 := N/\Omega \tag{9}$$

stands for the *total* concentration of the fermions, with N the *total* number of fermions in the system (see Eq. (20) below) and Ω the volume occupied by the system. For macroscopic systems, that is those in the thermodynamic limit corresponding to $N, \Omega \to \infty$ and n_0 a *finite* constant, the Hamiltonian $\widehat{H}_{\kappa}$ accounts for two contributions, namely the self-interaction energy of a positively charged uniform background of charge density $e n_0$, which is equal to $-\widehat{H}_{\kappa}$, and the interaction energy of the negatively charged fermions with the above-mentioned background, which is equal to $2\widehat{H}_{\kappa}$ (Fetter and Walecka 1971, pp. 21-23). [25] The prefactor 2 reflects the fact that here an energy of two mutually distinguishable systems of uniformly distributed particles is concerned; with each system containing N particles, there are N^2 distinct pairs of interactions, which is to be contrasted with the self-interaction energy of a system of (uniformly distributed) N particles for which there are $N(N-1)/2$ pairs of distinct interactions, which to the leading order in N for $N \to \infty$ is equal to $N^2/2$.

In the above results, κ, which has the dimension of reciprocal metres, has its root in the 'soft' cut-off function $\exp(-\kappa\|\boldsymbol{r}-\boldsymbol{r}'\|)$ with which $v_c(\boldsymbol{r}-\boldsymbol{r})$ in Eq. (4) has to be multiplied for the purpose of evaluating the electrostatic potential energies due to uniform charge distributions (see Eq. (13) below). In this connection, we note that

$$\int_{\Omega} \mathrm{d}^3 r' \; \frac{\exp(-\kappa\|\boldsymbol{r}-\boldsymbol{r}'\|)}{\|\boldsymbol{r}-\boldsymbol{r}'\|} \to \frac{4\pi}{\kappa^2} \;\; \text{for} \;\; \Omega \to \infty. \tag{10}$$

In arriving at this result we have made the *assumption* that $R \exp(-\kappa R)/\kappa \ll 1/\kappa^2$, where $R := a\Omega^{1/3}$ with a some finite positive constant (say, $a = (3/[4\pi])^{1/3}$), implying the condition $1/R \ll \kappa$. This signifies the fact that *in using the result in Eq. (5), $R \to \infty$ must be applied before taking the limit $\kappa \downarrow 0$.* In view of our later considerations, we point out that, in cases where one encounters the 'soft' cut-off $\exp(-\kappa\|\boldsymbol{r}-\boldsymbol{r}'\|)$, disregard for the condition $1/R \ll \kappa$ can lead to erroneous results, so that it is crucial to deal with integrals involving this cut-off function with sufficient care (see Appendix F, § 1.b herein). It is further important to realize that introduction of a cut-off function, such as $\exp(-\kappa\|\boldsymbol{r}-\boldsymbol{r}'\|)$, in conjunction with v_c, is *not* a mere regularization device, but serves to account for the fact that the interaction potential v_c mediates between two particles (of charge $-e$) described by square integrable wave functions (the totality of these functions constitutes the single-particle Hilbert space of the problem); this device thus enables one to introduce such gauge-non-invariant function as $\Sigma_{\sigma}(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ in complete isolation from the context in which it determines observable quantities (which are gauge invariant) where it is integrated with respect to $\boldsymbol{r}$, $\boldsymbol{r}'$ or $\boldsymbol{r}$ *and* $\boldsymbol{r}'$ together with functions that are square integrable over an unbounded space (see, e.g., Eq. (84) below).

In considering $\widehat{H}_{\kappa} + \widehat{H}$, with $\widehat{H}$ as defined in Eq. (1), we merely need to apply in Eq. (2) the substitution

$$u(\boldsymbol{r}) \rightharpoonup u(\boldsymbol{r}) - \varpi_{\kappa}, \tag{11}$$

on account of the definition for $\widehat{N}$ in Eq. (6) above. By decomposing, in *macroscopic* systems, the *total* number density $n(\boldsymbol{r})$ as follows

$$n(\boldsymbol{r}) = n_0 + n'(\boldsymbol{r}) \;\; \text{with} \;\; \int \mathrm{d}^d r \; n'(\boldsymbol{r}) = 0, \tag{12}$$

where n_0 is the total concentration of fermions, defined in Eq. (9), with

$$v'(\boldsymbol{r}-\boldsymbol{r}') := \begin{cases} v(\boldsymbol{r}-\boldsymbol{r}'), \\ \\ v_c(\boldsymbol{r}-\boldsymbol{r}')\, \mathrm{e}^{-\kappa\|\boldsymbol{r}-\boldsymbol{r}'\|}, \quad \kappa \downarrow 0, \end{cases} \tag{13}$$

for the electrostatic Hartree potential

$$v_H(\boldsymbol{r}; [n]) := \int \mathrm{d}^d r' \; v'(\boldsymbol{r}-\boldsymbol{r}')\, n(\boldsymbol{r}'), \tag{14}$$

which is a *linear* functional of n, in the case of $d = 3$ and $v \equiv v_c$ we have

$$v_H(\boldsymbol{r}; [n]) \equiv \varpi_{\kappa} + v_H(\boldsymbol{r}; [n']). \tag{15}$$

It is seen that ϖ_{κ} cancels in the sum of the *transformed* external potential, according to Eq. (11), and $v_H(\boldsymbol{r}; [n])$,

[25] Our formulation slightly differs from that by Fetter and Walecka (1971) who do *not* introduce $\widehat{H}_{\kappa}$ involving the total number *operator* $\widehat{N}$; they rather introduce the N-particle GS expectation value of what we have denoted by $\widehat{H}_{\kappa}$ which is sufficient so long as one does not need to deal with contributions to the SE operator beyond the first order in the particle-particle interaction.

according to Eq. (15) so that, upon adding the two potentials, κ can be set equal to zero. For completeness, for finite systems of fermions (such as atoms and molecules) interacting through the Coulomb potential, κ in Eq. (13) can be set equal to zero from the outset. *In the remaining part of this paper, unless we indicate or imply otherwise,* $v(\boldsymbol{r}-\boldsymbol{r}')$ *will denote* $v'(\boldsymbol{r}-\boldsymbol{r}')$ *as defined in Eq. (13).*

As we shall see later in this work, the property

$$\nabla^2_{\boldsymbol{r}}\, v_c(\boldsymbol{r}-\boldsymbol{r}') = \frac{-e^2}{\epsilon_0}\,\delta(\boldsymbol{r}-\boldsymbol{r}'), \qquad (16)$$

together with $v_c(\boldsymbol{r}-\boldsymbol{r}') \to \infty$ for $\|\boldsymbol{r}-\boldsymbol{r}'\| \to 0$ have far-reaching consequences for systems of fermions interacting through the two-body potential v_c. [26] This aspect is additional to that corresponding to the long range of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ for $\|\boldsymbol{r}-\boldsymbol{r}'\| \to \infty$ which is specific to macroscopic systems. [27] To clarify this statement, suffice it for the moment to mention that in some of the relevant expressions (see Eqs. (202) and (203) below), we will encounter terms involving $v(\boldsymbol{r}-\boldsymbol{r}')\tau(\boldsymbol{r})v(\boldsymbol{r}-\boldsymbol{r}')$, which, in view of Eqs. (3), (16) and (4), is unbounded for $v \equiv v_c$.

In the light of the above remarks, we should emphasize that the significance that we ascribe to the Coulomb potential in $d = 3$ should *not* be considered as implying that other two-body potentials than the Coulomb potential, and/or $d \neq 3$ were devoid of such significance. It is in fact possible to bring about even very peculiar results for arbitrary d by considering two-body potentials that are not necessarily physically feasible.

B. Some details concerning asymptotic series

Since in this work our main attention is focussed on AS expansions (Whittaker and Watson 1927, chapter VIII, Copson 1965, Dingle 1973, Murray 1974, Lauwerier 1977), here we briefly present some details concerning these.

An *asymptotic series* (AS) (in the sense of Poincaré [28]) is based on an *asymptotic sequence* (Lauwerier, 1977): $\{\tilde{\phi}_m(z)\|m = 0, 1, \dots\}$ is an asymptotic sequence corresponding to the asymptotic region $z \to z_0$ provided that $\tilde{\phi}_{m+1}(z)/\tilde{\phi}_m(z) \to 0$ for $z \to z_0$, which property is formally denoted by $\tilde{\phi}_{m+1}(z) = o\big(\tilde{\phi}_m(z)\big)$, for $z \to z_0$. In our present work, z_0 is the point of infinity in the complex z plane and $\{1, 1/z, 1/z^2, \dots\}$ the asymptotic sequence of our choice; thus, unless we indicate otherwise, in what follows z_0 will be the point of infinity.

For functions which are analytic outside a disc of finite radius centred around $z = 0$, the series in terms of $\{1/z, 1/z^2, \dots\}$ constitutes the *principal part* (as opposed to the *analytic part*) of the Laurent series of these functions; for functions which possess a pole of order m at $z = 0$ and are analytic elsewhere, the principal part of their corresponding Laurent series terminates at the mth term, corresponding to $1/z^m$; functions whose principal parts of their Laurent series do not terminate, must therefore possess a *non*-isolated singularity at $z = 0$. Through defining $\zeta{:=}1/z$ (which amounts to a conformal mapping), our AS would coincide with the Taylor series based upon $\zeta = 0$ if the functions under consideration were analytic in (finite) neighbourhoods of the origin in the ζ plane. As a Taylor series is a power series, its region of convergence in the complex plane is a circular disk, inside which (that is, excluding the boundary of the disk) it converges absolutely and uniformly. In contrast, an AS may not converge. [29] Consequently, AS, in particular those based on the asymptotic sequence $\{1, 1/z, 1/z^2, \dots\}$, concern a wider class of functions than those capable of being described by means of Taylor or Laurent series.

For definiteness, consider the function $\tilde{f}(z)$ as representing the functions dealt with in the present work, such as the coordinate representations of the single-particle Green *operator* $\widetilde{G}_\sigma(z)$ and of the associated SE *operator* $\widetilde{\Sigma}_\sigma(z)$ (see footnote 11). Further, consider the AS $\tilde{f}(z) \sim a_0 + a_1/z + a_2/z^2 + \dots$, with a_0, a_1, …, constants. By definition (according to Poincaré) we have $z^m\big(\tilde{f}(z) - \sum_{j=0}^m a_j/z^j\big) \to 0$ as $|z| \to \infty$, for $m \geq 0$. [30] It

[26] From Eqs. (14) and (16) one readily deduces $\nabla^2_{\boldsymbol{r}} v_H(\boldsymbol{r};[n]) = (-e^2/\epsilon_0)\, n'(\boldsymbol{r})$, with $n'(\boldsymbol{r})$ as defined in Eq. (12). The definiteness of this result depends on enforcing $\kappa = 0$ *subsequent to* evaluating $\nabla^2_{\boldsymbol{r}} v_H(\boldsymbol{r};[n])$ with $\kappa \neq 0$. Without this, one would *incorrectly* deduce $(-e^2/\epsilon_0)\, n(\boldsymbol{r})$ for the right-hand side of the latter expression.

[27] It is important, however, to realize that the two properties are *not* unrelated; both are associated with the fact that $v_c(\boldsymbol{r}-\boldsymbol{r}')$ is a *homogeneous* function (for example Ince 1927, p. 10) of degree minus unity, which is implicit in the expression in Eq. (16); with $\alpha > 0$, making use of the property $\delta(\alpha[\boldsymbol{r}-\boldsymbol{r}']) = \alpha^{-d}\delta(\boldsymbol{r}-\boldsymbol{r}')$, $d = 3$, from $\nabla^2_{\alpha\boldsymbol{r}} = \alpha^{-2}\nabla^2_{\boldsymbol{r}}$ it follows that for v_c satisfying Eq. (16), we must have $v_c(\alpha[\boldsymbol{r}-\boldsymbol{r}']) \equiv \alpha^{-1}\, v_c(\boldsymbol{r}-\boldsymbol{r}')$. This is indeed satisfied by v_c in Eq. (4).

[28] This restricted sense of AS (for details of the inherent restrictions of the Poincaré definition — as well as the extended Poincaré-Watson definition — see Dingle (1973)) is sufficient for our considerations in this paper. This follows from the fact that none of the functions of ε dealt with in this paper involves exponentially-decaying components for $|\varepsilon| \to \infty$ (see footnote 30 below).

[29] In fact, according to Whittaker and Watson (1927), (Chapter VIII), divergence of a series is a prerequisite for this to be considered as an AS.

[30] The restriction of the Poincaré definition is evident from the fact that $\sum_{j=1}^m a_j/z^j$ is unique up to exponentially-

is, however, possible that, for a given $\tilde{f}(z)$, the expression for a_m, for *some* m, involves an unbounded contribution (see later), which we denote by a_m^{u} and thus write $a_m = a_m^{\mathrm{u}} + a_m^{\mathrm{b}}$, where the bounded contribution a_m^{b} may or may not be vanishing. Considering the *ordered* set $\{a_j\}$ as being defined in terms of integrals, a_m^{u} can be viewed as corresponding to a non-integrable integrand. Let a_m be the first unbounded coefficient in the ordered set $\{a_j\}$. By *assuming* $\tilde{f}(z)$ to be a well-defined function, the *unbounded* contribution a_m^{u}/z^m, associated with a_m/z^m, in the AS $\tilde{f}(z) \sim a_0 + a_1/z + a_2/z^2 + \dots$ must be cancelled by equally unbounded contributions that *must* necessarily exist in the series $a_{m+1}/z^{m+1} + a_{m+2}/z^{m+2} + \dots$, corresponding to unbounded coefficients $\{a_j^{\mathrm{u}} \| j > m\}$. The latter set *cannot* be finite, for it is *not* possible to maintain the balance between the unbounded contributions of the form a_j^{u}/z^j, $j \ge m$, by means of a *finite* set of coefficients for z varying over an *open* region of the complex z plane, that is a neighbourhood of the point of infinity. Thus the series $\sum_{j=m}^{\infty} a_j^{\mathrm{u}}/z^j$, which for it to be meaningful must be viewed as representing an expression in which the summation over j is carried out *prior to* the explicit evaluation of each of a_j^{u}, [31] gives rise to a transcendental function of z which for $|z| \to \infty$ is asymptotically *more* dominant than a_m^{b}/z^m. This follows from the fact that the possibility of the asymptotic dominance of a_m^{b}/z^m with respect to $\sum_{j=m}^{\infty} a_j^{\mathrm{u}}/z^j$ would be tantamount to a_j^{u} being vanishing, which is a contradiction. Following the same line of reasoning, one arrives at the conclusion that $\sum_{j=m}^{\infty} a_j^{\mathrm{u}}/z^j$ is asymptotically *less* dominant than a_{m-1}/z^{m-1} for $|z| \to \infty$ (assuming $m \ge 1$). In this work, we encounter a situation where a_0 and a_1 are bounded, but a_2 contains an unbounded contribution a_2^{u}. The latter in turn consists of two contributions, $a_{2;1}^{\mathrm{u}}$ and $a_{2;2}^{\mathrm{u}}$ corresponding to two infinite sets $\{a_{2;1}^{\mathrm{u}}, a_{3;1}^{\mathrm{u}}, \dots\}$ and $\{a_{2;2}^{\mathrm{u}}, a_{3;2}^{\mathrm{u}}, \dots\}$ for which $\sum_{j=2}^{\infty} a_{j;1}^{\mathrm{u}}/z^j \sim A_{2;1} \ln(-z/\varepsilon_0)/z^2$ and $\sum_{j=2}^{\infty} a_{j;2}^{\mathrm{u}}/z^j \sim A_{2;2}(-z/\varepsilon_0)^{1/2}/z^2$ hold, for $|z| \to \infty$. Note that, in the asymptotic region $|z| \to \infty$, both $\ln(-z/\varepsilon_0)/z^2$ and $(-z/\varepsilon_0)^{1/2}/z^2$ are indeed *more* dominant [32] than $1/z^2$ and *less* dominant than $1/z$, in full conformity with our above general statement.

The above discussions bring out one essential aspect related to *finite*-order AS, namely that *in general* deducing these through merely truncating an infinite-order (asymptotic) series (we refer to these as '*formal* finite-order AS'), gives rise to ill-defined functions and that derivation of meaningful finite-order AS may require partial summations of some infinite number of terms in the original infinite series. Unless implied by the context otherwise, our explicit references in this work to 'finite-order asymptotic series' concern the well-defined (or regularized) AS consisting of finite number of terms.

A point of considerable importance to our investigations in this paper is the following. Consider

$$\tilde{f}(\boldsymbol{r}; z) := \int \mathrm{d}^d r' \; \tilde{g}(\boldsymbol{r}, \boldsymbol{r}'; z)$$

and suppose that

$$\tilde{g}(\boldsymbol{r}, \boldsymbol{r}'; z) \sim \gamma_0(\boldsymbol{r}, \boldsymbol{r}') + \frac{\gamma_1(\boldsymbol{r}, \boldsymbol{r}')}{z} + \dots, \;\; \text{for } \; |z| \to \infty.$$

From our above discussions it follows that with

$$\phi_j(\boldsymbol{r}) := \int \mathrm{d}^d r' \; \gamma_j(\boldsymbol{r}, \boldsymbol{r}'),$$

$$\tilde{f}(\boldsymbol{r}; z) \sim \sum_{j=0}^{m} \frac{\phi_j(\boldsymbol{r})}{z^j}$$

is the AS with respect to the asymptotic sequence $\{1, 1/z, \dots\}$ of $\tilde{f}(\boldsymbol{r}; z)$, for $|z| \to \infty$, involving the complete $m+1$ *leading* terms, provided that the integrals in terms of which the functions $\phi_j(\boldsymbol{r})$, $j = 0, 1, \dots, m$, are defined are bounded almost everywhere, that is bounded with the exception of a possible *finite* set of $\boldsymbol{r}$ points (see further; for periodic systems, the latter set of $\boldsymbol{r}$ points concerns those in the primitive cell). Here it is important to note the *sufficiency* of *boundedness* of the integrals defining $\phi_j(\boldsymbol{r})$, $j = 0, 1, \dots, m$, for the validity of the latter statement. With reference to our above considerations, the possibility of *non*-integrability of $\gamma_{m+1}(\boldsymbol{r}, \boldsymbol{r}')$ with respect to $\boldsymbol{r}'$ (for almost *all* $\boldsymbol{r}$) implies that the most

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decaying functions of z. In general, such exponential functions exist and play a crucial role in compensating for the Stokes discontinuities in asymptotic expansions of continuous functions on crossing the Stokes rays (see Dingle 1973); note in passing that these rays concern discontinuities in the *form*, as opposed to those in the summed values, of these expansions (for example Morse and Feshbach (1953, p. 609)).

[31] One may think of a_j^{u}, $j \ge m$, as being defined in terms of integrals of bounded integrands, so that the unboundedness of these coefficients must be because these integrands are not integrable; the assumption with regard to the boundedness of $\sum_{j=m}^{\infty} a_m^{\mathrm{u}}/z^m$ is therefore a statement with regard to the integrability of the complete sum of the integrands associated with a_j^{u}/z^j, $j \ge m$. Here the transcendental function $z^m \sum_{j=m}^{\infty} a_j^{\mathrm{u}}/z^j$ *may* or *may not* involve a non-vanishing z-*in*dependent part; in cases it does, one could re-define a_m^{b} by absorbing this z-independent part into it so that *by definition* $z^m \sum_{j=m}^{\infty} a_j^{\mathrm{u}}/z^j$ would be without a z-independent contribution. In this paper we do *not* adopt such redefinition. See, for instance, Section 5.b in Appendix F.

[32] For more general AS than those according to the Poincaré definition, 'more dominant' does *not* necessarily imply 'decaying less fast'. See the main text as well as footnote 126.

leading asymptotic term following $\phi_m(\boldsymbol{r})/z^m$ must decay either more *slowly* than $1/|z|^{m+1}$ or as slowly as $1/|z|^m$, but with increasingly rapidly oscillatory behaviour as $|z| \to \infty$; for instance, with $z = \varepsilon$, one may encounter a function of the form $\cos(\varepsilon/\varepsilon_0 + \vartheta)/\varepsilon^m$, with ε_0 a constant energy and ϑ a constant phase. [33] Considerations involving AS of this nature lie outside the scope of the Poincaré formalism and further will not concern us in this paper (see footnote 28) so that, in the context of our considerations in this paper, the term following $\phi_m(\boldsymbol{r})/z^m$ necessarily should decay more *slowly* than $1/|z|^{m+1}$ when $\gamma_{m+1}(\boldsymbol{r}, \boldsymbol{r}')$ is non-integrable with respect to $\boldsymbol{r}'$ for almost *all* $\boldsymbol{r}$.

In this work we shall be dealing with systems in which particles interact through, in principle, arbitrary potentials $v(\boldsymbol{r}-\boldsymbol{r}')$ and $u(\boldsymbol{r})$, with each other and with a background respectively. As is the case with the Coulomb potential in $d = 3$, $v(\boldsymbol{r} - \boldsymbol{r}')$ can increase *indefinitely* for $\|\boldsymbol{r} - \boldsymbol{r}'\| \to 0$, and similarly can $|u(\boldsymbol{r})|$ increase indefinitely for $\|\boldsymbol{r} - \boldsymbol{R}_j\| \to 0$, where $\{\boldsymbol{R}_j\}$ denotes the set of position vectors of the atomic nuclei in the system (see Appendix K). Both because of these and owing to the unboundedness of the kinetic-energy operator (for example Kreyszig (1978, chapter 10)), [34] we are confronted with a situation where in principle the problem has *no a priori* high-energy scale which is required for the notion 'large $|\varepsilon|$' to have a precise meaning. [35] This aspect is clearly illustrated by considering an example, taken from § III.H (see also Appendix H), where in what we call 'the large-$|z|$ asymptotic series' for the SE operator in the coordinate representation, $\widetilde{\Sigma}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$ (see Eqs. (62) and (72) below), we encounter the sequence (see Eqs. (173), (185) and (199); see also Eq. (212))

$$\big\{v^m(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}', \boldsymbol{r})/z^{m-1} \| m = 1, 2, \dots\big\}.$$

Assuming v to be the Coulomb potential v_c in $d = 3$, it is seen that whatever large finite value is assigned to $|z|$, by decreasing $\|\boldsymbol{r} - \boldsymbol{r}'\|$ beyond a certain z-dependent limit, the terms in this sequence, in the order presented, can be made to *increase* in amplitude rather than to decrease, in evident contradiction with the perception that one may have of AS (see later). Irrespective of whether such understanding of AS is correct or not (it is *not*, as we shall discuss below), this example brings out the mechanism by which in particular the short-range part of the Coulomb interaction potential stands in the way of introducing an *a priori* high-energy scale in the context of the AS expansion of $\Sigma_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ for $|\varepsilon| \to \infty$.

The 'perception' with regard to AS, to which we have referred above, is *false*. This is directly established by realizing the fact that AS are named such by the very aspect of being a series *in terms of* an *asymptotic sequence* appropriate to some asymptotic region. In fact, if the terms in an AS had to be monotonically decreasing in magnitude, by the D'Alembert criterion all AS would have to be absolutely convergent in sufficiently small but non-vanishing neighbourhoods of the asymptotic point. As we have indicated at the outset of this Section (see footnote 29), however, the authoritative text by Whittaker and Watson (1927, chapter VIII) explicitly reserves the designation 'asymptotic series' for those which, *in addition to* being asymptotic in the sense just indicated, are also divergent (see also Dingle (1973)). [36] For clarity, consider the series $\sum_{m=0}^{\infty}(-1)^m m! z^m$, which is divergent for *any* non-vanishing z; from the D'Alembert criterion, it follows that, for this series to be convergent, it is necessary that $|z| \le 1/(m+1)$ as $m \to \infty$. This series can however be summed by means of the Borel, or Euler, summation technique (for example Lauwerier (1977)), resulting in (Farid 1999c) $\exp(1/z)\mathrm{E}_1(1/z)/z =: \tilde{f}(z)$, where $\mathrm{E}_1(\zeta)$ stands for the exponential-integral function (Abramowitz and Stegun 1972, p. 228) (see also Appendix I for some relevant details); any finite-order truncation of the above

[33] Recall that $\cos(z)$ is a transcendental function of z.

[34] In many practical calculations, through imposing ultraviolet (or large-momentum) cut-offs, the unbounded character of the kinetic-energy operator is suppressed. This is specifically the case in the conventional Hubbard model (for example Montorsi (1992), Gebhard (1997)) where the ultraviolet cut-off is implied by the finite number of (non-interacting) bands (or finite number of orbitals per lattice point) taken into account.

[35] Later in this Section we specify how in practice an appropriate energy scale can be identified with respect to which $|\varepsilon|$ can be considered as large.

[36] In fact, in contrast with Taylor series and the principal parts of Laurent series which may be considered as being AS in terms of the asymptotic sequences $\{1, z, z^2, \dots\}$ and $\{1/z, 1/z^2, \dots\}$ appropriate to the asymptotic points $z = 0$ and $1/z = 0$ respectively, and whose convergence for a particular z in a neighbourhood of these points, say $z = z_0$, implies their convergence for *all* $z = |z_0|\exp(i\varphi)$, $\varphi \in [0, 2\pi]$, *asymptotic* series are in general associated with functions that do *not* admit such *uniform* representations as Taylor and Laurent series. Consider for instance $\tilde{f}(z)$ which we assume to be bounded in a neighbourhood of $z = z_0$. The AS $\tilde{f}(z) \sim f_0 + f_1(z - z_0) + f_2(z - z_0)^2 + \dots$, for $z \to z_0$, either converges when $|z - z_0| < \eta$ for *some* positive η (in which case it converges uniformly), or it diverges for *any* positive η. The latter divergence signals the non-analyticity of $\tilde{f}(z)$ at $z = z_0$; z_0 is for instance a branch point of $\tilde{f}(z)$. Consequently, the neighbourhood of z_0 can be subdivided into a number of sectors in each of which $\tilde{f}(z)$ admits an AS specific to that sector. Consider (Lauwerier 1977, p. 11) $\tilde{f}(z) := \exp(z) + \exp(-z)\tanh(1/z)$ which has the following AS for $z \to 0$: $\tilde{f}(z) \sim 2\cosh(z) \sim 2 + z^2 + \dots$, for $\mathrm{Re}(z) > 0$, and $\tilde{f}(z) \sim 2\sinh(z) \sim 2z + z^3/3 + \dots$, for $\mathrm{Re}(z) < 0$.

series is an AS (with respect to the asymptotic sequence $\{1, z, z^2, \dots\}$) of $\tilde{f}(z)$ for $|z| \to 0$, with $-\pi < \arg(z) < \pi$.

In spite of the above, it remains worth enquiring whether an AS for the SE operator corresponding to $|z| \to \infty$, possessing the peculiarities associated with $\|\boldsymbol{r} - \boldsymbol{r}'\| \to 0$ considered above, can be of *physical* relevance. It is further of significance to know the energy scale beyond which a finite-order AS for the SE operator corresponding to $|z| \to \infty$ can be considered as being an accurate representation of the exact $\widetilde{\Sigma}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$. Below we shall briefly address these two issues.

— Firstly, the peculiarity concerning the short-distance behaviour of the coefficients in the large-$|z|$ AS for $\widetilde{\Sigma}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$, pertaining to systems of Coulomb-interacting particles, is *partly* (see later) an aspect specific to the coordinate representation of $\widetilde{\Sigma}_\sigma(z)$, which gives, by its very nature, prominence to the behaviour of this *operator* on *all* length scales; such indiscriminate representation [37] is physically non-essential for the SE operator which is not gauge invariant and therefore not an observable. Observable quantities, insofar as they are determined by $\widetilde{\Sigma}_\sigma(z)$, such as the single-particle excitation *energies* (see § III.D), involve matrix elements of $\widetilde{\Sigma}_\sigma(z)$ with respect to a set of basis functions spanning the single-particle Hilbert space of the system under consideration (contrast this with the matrix elements of $\widetilde{\Sigma}_\sigma(z)$ with respect to $|\boldsymbol{r}\rangle$ and $|\boldsymbol{r}'\rangle$; see footnote 37). Expressing the latter matrix elements in terms of integrals of $\widetilde{\Sigma}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$ and the coordinate representation of the pertinent basis functions (*cf.* Eq. (84) below), one observes that a finite-order AS for $\widetilde{\Sigma}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$, $|z| \to \infty$, is unequivocally well-defined provided its constituent functions the following hold true.

(A) They are bounded (more precisely, bounded almost everywhere).

(B) They are integrable (here, in the sense of Riemann) with respect to $\boldsymbol{r}$ (or, equivalently, $\boldsymbol{r}'$, since $\widetilde{\Sigma}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$ is symmetric with respect to $\boldsymbol{r} \rightleftharpoons \boldsymbol{r}'$) over *any finite* region of the single-particle configuration space.

(C) Also, for systems in the thermodynamic limit, they decay sufficiently rapidly at large distances from the origin, so that the pertinent integrals (see (B)) converge to finite values as the size of the system is made to approach infinity.

From these requirements it follows that, for $v \equiv v_c$ in $d = 3$, the terms $v_c^m(\boldsymbol{r} - \boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}', \boldsymbol{r})/z^{m-1}$, presented above, corresponding to $m = 1, 2$ are unreservedly well defined in a finite-order large-$|z|$ AS for $\widetilde{\Sigma}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$, but further terms, corresponding to $m > 2$, are *not*. We note in passing that this is the aspect to which we referred above through our use of the word 'partly'; the non-integrability of terms $v_c^m(\boldsymbol{r} - \boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}', \boldsymbol{r})/z^{m-1}$ for $m > 2$, though an aspect of the coordinate representation of the pertinent operators, reflects the fact that, in the case at hand and in the momentum representation, the contributions to the SE operator immediately following those decaying like $1/z$, are *not* those decaying like $1/z^2$, but some which decay more *slowly* than this (but *rapidly* than $1/|z|$). The *total* contribution of the sequence of non-integrable terms $\{v_c^m(\boldsymbol{r} - \boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}', \boldsymbol{r})/z^{m-1} \,\|\, m = 3, 4, \dots\}$ is directly seen to be equal to $z^{-2} v_c^3(\boldsymbol{r} - \boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}', \boldsymbol{r})/[1 - v_c(\boldsymbol{r} - \boldsymbol{r}')/z]$, which is indeed an integrable function of $\boldsymbol{r}$ and $\boldsymbol{r}'$. As we demonstrate in Appendix H, the momentum representation of the latter function involves a term proportional to $\ln(-z/\varepsilon_0)/z^2$, where ε_0 stands for a constant energy, followed by one proportional to $1/z^2$.

— Secondly, considering for the moment a bounded and short-range interaction potential v, a close inspection of the explicit expressions for the coefficient functions $\Sigma_{\sigma;\infty_m}(\boldsymbol{r}, \boldsymbol{r}')$ corresponding to $m = 0, 1, 2$ (see §§ III.F, III.G and III.H; see also Eq. (72) below for the definition), reveals that $\Sigma_{\sigma;\infty_0}(\boldsymbol{r}, \boldsymbol{r}')$ and $\Sigma_{\sigma;\infty_1}(\boldsymbol{r}, \boldsymbol{r}')$ are *explicitly* proportional to the first and the second powers respectively of the coupling constant of the particle-particle interaction; *higher-order coefficients* $\Sigma_{\sigma;\infty_m}(\boldsymbol{r}, \boldsymbol{r}')$*, corresponding to* $m \geq 2$*, are determined by a complex interplay between the interaction and the kinematics of the interacting particles, manifesting itself in a range of contributions which depend on all powers of the coupling constant of interaction from* 2 *up to and including* $m+1$ (*cf.* Eqs. (107)-(109) below). The latter aspect follows from the fact that the large-$|z|$ AS for $\widetilde{\Sigma}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$ amounts to an ordering of interaction effects in accordance with powers of $1/z$ associated with them rather than powers of the coupling constant of interaction which corresponds to the ordering scheme of the many-body perturbation theory. To be explicit, a general term in the expression for $\Sigma_{\sigma;\infty_m}$, pertaining to a system described by the Hamiltonian in Eqs. (1) and (2), involves p_1 times τ, p_2 times u and p_3 times v (all in various orders), with p_1, p_2 and p_3 constrained by the condition $p_1 + p_2 + p_3 = m + 1$; in the case of $m = 0$, by necessity we have $p_1 = p_2 = 0$, whereas since the first-order SE contributions in terms of v are static and can therefore only contribute to $\Sigma_{\sigma;\infty_0}$, and since v is a *two*-particle interaction function, for $m \geq 1$, $p_3 \geq 2$ (see, for example, Eqs. (107), (108) and (109) below).

In the specific case where $v \equiv v_c$ in $d = 3$ and for $m = 0, 1$, the dependences of $\Sigma_{\sigma;\infty_m}(\boldsymbol{r}, \boldsymbol{r}')$ on the coupling constant of interaction are the same as for bounded and short-range interaction potentials v discussed above;

[37] In this context it is important to recall that $\{|\boldsymbol{r}\rangle\}$ are the eigenstates of the *unbounded* $\hat{\boldsymbol{r}}$ operator which are δ function normalized, that is $\langle \boldsymbol{r}|\boldsymbol{r}'\rangle = \delta(\boldsymbol{r} - \boldsymbol{r}')$.

for $m \geq 2$ however, where $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ involves *fundamentally unbounded* contributions (it also involves *non-integrable* contributions whose regularization becomes necessary for the determination of the momentum representation of $\Sigma_{\sigma;\infty_m}$; see conditions (A) - (C) introduced and discussed above), on regularizing these, the dependence on the coupling constant of interaction of the regularized $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, which we denote by $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'|\varepsilon)$ (see § III.E.2), is no longer polynomial, but transcendental; as we show in § III.H, $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'|\varepsilon)$ involves the logarithm of this coupling constant (see, e.g., Eq. (114) below; we note in passing that the dependence of the right-hand side (RHS) of Eq. (113) on the logarithm of the coupling constant of interaction has its origin in the regularization of the aforementioned *non-integrable* contribution in $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$).

In metallic systems, the spherical average of the radius of the Fermi surface, k_F, defines the length-scale $\ell_F{:=}1/k_F$ relevant to the low-temperature transport and thermodynamic properties of these systems. Consequently, for these systems, $\hbar\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ should be proportional to $(g/\ell_F)^{m+1}$ for $m = 0, 1$, where g stands for the coupling-constant of the particle-particle interaction; for $v \equiv v_c$ in $d = 3$ we have $g = g_c \equiv e^2/(4\pi\epsilon_0)$ so that, using $k_F = (3\pi^2 n_0)^{1/3}$, applicable to systems with simply-connected Fermi-surface geometries (here n_0 denotes the average total electron concentration; see Eq. (9) above), we deduce the energy scale $e^2/(4\pi\epsilon_0\ell_F){=:}e_0'$ to be on the order of 2 Hartrees or less (1 Hartree = 2 Rydberg $\approx$ 27.21 eV); for Sodium, for instance, this scale is $\frac{1}{2}$ Hartree (for a precise formulation see § III.E and in particular § III.E.4). For these systems, on this scale of energies, $\hbar\Sigma_{\sigma;\infty_1}/\varepsilon$ should become comparable with $\Sigma_{\sigma;\infty_0}$. In § III.E where we introduce the formalism appropriate for dealing with uniform and isotropic GSs, we provide a quantitative analysis of the result given here and further determine the role played by contributions in the AS for the SE that decay more rapidly than $1/\varepsilon$ for $|\varepsilon| \to \infty$. However, irrespective of these quantitative results, it would be quite mistaken to assess the utility of a finite-order AS for $\widetilde{\Sigma}_\sigma(z)$ corresponding to $|z| \to \infty$ solely in terms of the accuracy with which it describes the exact $\widetilde{\Sigma}_\sigma(z)$ at sufficiently large values of $|z|$. As we discuss in § III.B in some detail, such series, when exact to order m in $1/z$, lead to the *exact* large-$|z|$ AS of the single-particle GF $\widetilde{G}_\sigma(z)$ to all orders up to and including $m+2$ in $1/z$. [38] This in turn implies, via Eqs. (37) and (38), that the energy moment integrals of the corresponding single-particle spectral function are exact to order $m+1$ (see footnote 6). In other words, insofar as a particular finite-order energy moment integral of the single-particle spectral function is concerned (for definitions see Eqs. (37) and (38) below), it is entirely *immaterial* whether or not (if at all), in a finite-order AS for $\widetilde{\Sigma}_\sigma(z)$, the terms beyond a certain order in $1/z$ are properly taken into account. In § III.E.6, after having explicitly introduced some of the necessary ingredients that are essential to our present work, we clarify the above statements by means of a simple example concerning uniform and isotropic systems of fermions.

[38] From the Dyson equation one obtains $\widetilde{G}_\sigma(z) = \big(I - G_{0;\sigma}(z)\Sigma_\sigma(z)\big)^{-1} G_{0;\sigma}(z) = \widetilde{G}_{0;\sigma} + \widetilde{G}_{0;\sigma}(z)\widetilde{\Sigma}_{0;\sigma}(z)\widetilde{G}_{0;\sigma}(z) + \dots$. The fact that $\widetilde{\Sigma}_\sigma(z)$ is 'sandwiched' between at least *two* $\widetilde{G}_{0;\sigma}(z)$ functions, with $\widetilde{G}_{0;\sigma}(z) \sim \hbar I/z$ for $|z| \to \infty$ (see Eq. (61)), underlies the 2 in $m+2$.

III. THEORY

A. Generalities

Our starting point in this work is the Lehmann (1954) spectral representation for the single-particle GF corresponding to the N-particle GS (which we assume to be non-degenerate and *normal*, i.e. with *no* off-diagonal long-range order; for definition see Reichl (1980)) of a system of spin-s fermions, with s *any* half-integer:

$$G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon) = \hbar \sum_s f_{s;\sigma}(\boldsymbol{r}) f^*_{s;\sigma}(\boldsymbol{r}') \times \left\{ \frac{\Theta(\mu - \varepsilon_{s;\sigma})}{\varepsilon - \varepsilon_{s;\sigma} - i\eta} + \frac{\Theta(\varepsilon_{s;\sigma} - \mu)}{\varepsilon - \varepsilon_{s;\sigma} + i\eta} \right\},\ \eta \downarrow 0, \quad (17)$$

where $\{f_{s;\sigma}(\boldsymbol{r})\}$ are the 'Lehmann amplitudes' defined by

$$f_{s;\sigma}(\boldsymbol{r}) := \begin{cases} \langle \Psi_{N_\sigma-1,N_{\bar\sigma};s} | \hat{\psi}_\sigma(\boldsymbol{r}) | \Psi_{N;0} \rangle, & \varepsilon_{s;\sigma} < \mu, \\ \langle \Psi_{N;0} | \hat{\psi}^\dagger_\sigma(\boldsymbol{r}) | \Psi_{N_\sigma+1,N_{\bar\sigma};s} \rangle, & \varepsilon_{s;\sigma} > \mu, \end{cases} \quad (18)$$

and

$$\varepsilon_{s;\sigma} := \begin{cases} E_{N;0} - E_{N_\sigma-1,N_{\bar\sigma};s}, & \varepsilon_{s;\sigma} < \mu, \\ E_{N_\sigma+1,N_{\bar\sigma};s} - E_{N;0}, & \varepsilon_{s;\sigma} > \mu, \end{cases} \quad (19)$$

are the single-particle excitation energies; here μ stands for the 'chemical potential' (see text following Eq. (22) below). With $\bar\sigma$ denoting the *set* of $2\mathsf{s}$ spin indices complementary to σ, throughout this work we consider

$$N = N_\sigma + N_{\bar\sigma}, \quad (20)$$

where

$$N_{\bar\sigma} := \sum_{\sigma' \neq \sigma} N_{\sigma'}. \quad (21)$$

In Eq. (18), $|\Psi_{M_\sigma,M_{\bar\sigma};s}\rangle$ denotes a simultaneous *normalized* eigenstate of the many-body Hamiltonian $\widehat{H}$, with

$E_{M_\sigma,M_{\bar\sigma};s}$ the corresponding eigen-energy, [39] and the *partial* number operators $\widehat{N}_\sigma$, $\sigma = -\mathsf{s}, -\mathsf{s}+1, \dots, \mathsf{s}$, defined in Eq. (7), with $\{M_\sigma\}$, the corresponding eigen-numbers; in Eqs. (18) and (19), we have specifically employed the short-hand notations $|\Psi_{N;s}\rangle \equiv |\Psi_{N_\sigma,N_{\bar\sigma};s}\rangle$ and $E_{N;s} \equiv E_{N_\sigma,N_{\bar\sigma};s}$.

Above, s is a compound variable which consists of all indices that characterize the pertinent eigenstates of $\widehat{H}$ (see text following Eq. (44) below and footnotes 50 and 109), with $s = 0$ reserved to *symbolize* the non-degenerate GS of the system. Further, μ denotes the "chemical potential", satisfying

$$\mu_{N;\sigma}^{-} < \mu < \mu_{N;\sigma}^{+}, \quad \sigma \in \{-\mathsf{s}, -\mathsf{s}+1, \dots, \mathsf{s}\}, \tag{22}$$

where

$$\begin{aligned} \mu_{N;\sigma}^{-} &:= E_{N;0} - E_{N_\sigma-1,N_{\bar\sigma};0}, \\ \mu_{N;\sigma}^{+} &:= E_{N_\sigma+1,N_{\bar\sigma};0} - E_{N;0}. \end{aligned} \tag{23}$$

The existence of a μ which satisfies Eq. (22) is implied by the requirement of stability of the GS of the system (see footnote 60). In fact, $\mu_{N;\sigma}^{-}$ is independent of σ, that is it takes on the same value for *all* σ for which $N_\sigma \neq 0$ holds.

For our following considerations it is advantageous to introduce the analytic continuation of $G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ into the *physical* Riemann sheet of the z plane (see Farid 1999c); by doing so, no need will arise to deal separately with retarded and advanced GFs. Denoting the analytically continued function by $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$, for $\mathrm{Im}\{z\} \neq 0$ we have

$$\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z) = \hbar \sum_s \frac{f_{s;\sigma}(\boldsymbol{r}) f_{s;\sigma}^*(\boldsymbol{r}')}{z - \varepsilon_{s;\sigma}}, \tag{24}$$

from which the physical $G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ as presented in Eq. (17) is deduced according to

$$G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon) \equiv \lim_{\eta\downarrow 0} \widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon \pm i\eta), \quad \varepsilon \gtrless \mu. \tag{25}$$

We note in passing that for $\mathrm{Im}(z) \neq 0$, $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ satisfies the reflection property (Luttinger 1961, Farid 1999a,c, second paragraph of Appendix B)

$$\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z^*) \equiv \widetilde{G}_\sigma^*(\boldsymbol{r},\boldsymbol{r}';z). \tag{26}$$

The asymptotic expansion (see § II.B) of $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ for $|z| \to \infty$ (in the Poincaré sense) in terms of the asymptotic sequence $\{1/z^m \| m = 0,1,2,\dots\}$ is obtained by formally assuming an upper bound [40] to the absolute value of the single-particle energies $\{\varepsilon_{s;\sigma}\}$. For any $|z|$ greater than this upper bound, one obtains from Eq. (24) the following uniformly convergent series

$$\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z) = \sum_{m=1}^{\infty} \frac{G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')}{z^m}, \tag{27}$$

where

$$G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}') := \hbar \sum_s \varepsilon_{s;\sigma}^{m-1}\, f_{s;\sigma}(\boldsymbol{r}) f_{s;\sigma}^*(\boldsymbol{r}'), \quad m = 1,2,\dots. \tag{28}$$

These are *distributions* (Gelfand and Shilov 1964), as opposed to *functions*, as can be deduced from the following consideration: [41] making use of the definitions for the Lehmann amplitudes in Eq. (18) and the canonical equal-time anticommutation (Fetter and Walecka 1971) relations

$$\begin{aligned} \big[\hat\psi_\sigma^\dagger(\boldsymbol{r}), \hat\psi_{\sigma'}(\boldsymbol{r}')\big]_+ &= \delta_{\sigma,\sigma'}\, \delta(\boldsymbol{r}-\boldsymbol{r}'), \\ \big[\hat\psi_\sigma^\dagger(\boldsymbol{r}), \hat\psi_{\sigma'}^\dagger(\boldsymbol{r}')\big]_+ &= \big[\hat\psi_\sigma(\boldsymbol{r}), \hat\psi_{\sigma'}(\boldsymbol{r}')\big]_+ = 0, \end{aligned} \tag{29}$$

where $[\widehat{A},\widehat{B}]_+ := \widehat{A}\widehat{B} + \widehat{B}\widehat{A}$, one readily obtains

$$\begin{aligned} G_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}') &\equiv \hbar \sum_s f_{s;\sigma}(\boldsymbol{r}) f_{s;\sigma}^*(\boldsymbol{r}') \\ &= \hbar \sum_s \langle\Psi_{N;0}|\hat\psi_\sigma^\dagger(\boldsymbol{r}')|\Psi_{N_\sigma-1,N_{\bar\sigma};s}\rangle \\ &\qquad \times \langle\Psi_{N_\sigma-1,N_{\bar\sigma};s}|\hat\psi_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle \\ &\quad + \hbar \sum_s \langle\Psi_{N;0}|\hat\psi_\sigma(\boldsymbol{r})|\Psi_{N_\sigma+1,N_{\bar\sigma};s}\rangle \\ &\qquad \times \langle\Psi_{N_\sigma+1,N_{\bar\sigma};s}|\hat\psi_\sigma^\dagger(\boldsymbol{r}')|\Psi_{N;0}\rangle \\ &= \hbar \langle\Psi_{N;0}|\hat\psi_\sigma^\dagger(\boldsymbol{r}')\hat\psi_\sigma(\boldsymbol{r}) + \hat\psi_\sigma(\boldsymbol{r})\hat\psi_\sigma^\dagger(\boldsymbol{r}')|\Psi_{N;0}\rangle \\ &\equiv \hbar \langle\Psi_{N;0}|\big[\hat\psi_\sigma(\boldsymbol{r}), \hat\psi_\sigma^\dagger(\boldsymbol{r}')\big]_+|\Psi_{N;0}\rangle \\ &\equiv \hbar\delta(\boldsymbol{r}-\boldsymbol{r}'), \end{aligned} \tag{30}$$

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[39] We point out that our use of the word 'eigen-energy', which in a broader context would have been 'eigen-value', is suggestive that $\widehat{H}$ possesses a 'point spectrum', which for systems with continuous degrees of freedom is incorrect. In general, the *spectrum* of an operator is defined in terms of its associated *resolvent operator* (here $\widetilde{G}_\sigma(z)$) and can be grouped into three *disjoint* sets of *a point spectrum* (i.e. *eigenvalues*), *a continuous spectrum* and *a residual spectrum*. For a detailed discussion see the sections on the spectral theory in normed spaces in, for instance, Kreyszig (1978) and Debnath and Mikusiński (1990). For discussions concerning the relevance of the resolvent operator and its definition in terms of the Stieltjes integral, see the book by von Neumann (1955). See also footnote 2. In our considerations in this work, the set $\{s\}$ is assumed to exhaust the complete spectral contents of $\widehat{H}$.

[40] This upper bound E is made explicit in Eq. (38) below.

[41] These *distributions* can viewed as being the limits of *functions* $G_{\sigma;\infty_m}^{(E)}(\boldsymbol{r},\boldsymbol{r}')$, defined in Eq. (38), for $E \to \infty$.

which at the same time amounts to a statement concerning the completeness, or closure, [42] of the Lehmann amplitudes. Thus already $G_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ is a distribution. In arriving at Eq. (30) we have made use of the completeness of $\{|\Psi_{N_\sigma\pm1,N_{\bar\sigma};s}\rangle\}$ in the Hilbert space consisting of the direct product of the Hilbert spaces of $(N_\sigma\pm1)$- and $N_{\bar\sigma}$-particle states, that is

$$\sum_s |\Psi_{N_\sigma\pm1,N_{\bar\sigma};s}\rangle\langle\Psi_{N_\sigma\pm1,N_{\bar\sigma};s}| = \mathcal{I}_\sigma^{\pm}, \tag{31}$$

where $\mathcal{I}_\sigma^{\pm}$ stands for the unit operator in the abovementioned Hilbert space.

We point out that $\{f_{s;\sigma}(\boldsymbol{r})\}$ is *not* an orthogonal set, however reduces to an *orthonormal* set as the coupling constant of the particle-particle interaction is set equal to zero (see Eqs. (46) and (47) below; see also Appendix A). We further point out that $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, $m=1,2,\dots$, are c-numbers. As we shall see in the subsequent sections, the explicit expressions for $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, in particular those concerning $m=2,3,4$, that are encountered in our explicit calculations involve gradient operators so that this knowledge with regard to the c-number nature of these distributions informs us that these differential operators act on the functions involved in the explicit expression for $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ and *not* those exterior to it.

From Eq. (28), making use of Eqs. (18) and (19), we have

$$\begin{aligned} G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') &= \hbar\sum_s (E_{N;0}-E_{N_\sigma-1,N_{\bar\sigma};s})\\ &\times\langle\Psi_{N;0}|\hat\psi_\sigma^\dagger(\boldsymbol{r}')|\Psi_{N_\sigma-1,N_{\bar\sigma};s}\rangle\langle\Psi_{N_\sigma-1,N_{\bar\sigma};s}|\hat\psi_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle\\ &+\hbar\sum_s (E_{N_\sigma+1,N_{\bar\sigma};s}-E_{N;0})\\ &\times\langle\Psi_{N;0}|\hat\psi_\sigma(\boldsymbol{r})|\Psi_{N_\sigma+1,N_{\bar\sigma};s}\rangle\langle\Psi_{N_\sigma+1,N_{\bar\sigma};s}|\hat\psi_\sigma^\dagger(\boldsymbol{r}')|\Psi_{N;0}\rangle. \end{aligned} \tag{32}$$

Making use of $E_{M_\sigma,M_{\bar\sigma};s}|\Psi_{M_\sigma,M_{\bar\sigma};s}\rangle = \widehat{H}|\Psi_{M_\sigma,M_{\bar\sigma};s}\rangle$ and employing the completeness relation in Eq. (31), we readily obtain

$$\begin{aligned} G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') &= -\hbar\langle\Psi_{N;0}|\big[\widehat{H},\hat\psi_\sigma(\boldsymbol{r})\big]_-\hat\psi_\sigma^\dagger(\boldsymbol{r}')|\Psi_{N;0}\rangle\\ &\quad-\hbar\langle\Psi_{N;0}|\hat\psi_\sigma^\dagger(\boldsymbol{r}')\big[\widehat{H},\hat\psi_\sigma(\boldsymbol{r})\big]_-|\Psi_{N;0}\rangle\\ &\equiv\hbar\langle\Psi_{N;0}|\Big[\big[\hat\psi_\sigma(\boldsymbol{r}),\widehat{H}\big]_-,\hat\psi_\sigma^\dagger(\boldsymbol{r}')\Big]_+|\Psi_{N;0}\rangle, \end{aligned} \tag{33}$$

in which $[\widehat{A},\widehat{B}]_- {:=} \widehat{A}\widehat{B}-\widehat{B}\widehat{A}$ denotes commutation.

The expressions in Eqs. (30) and (33) suggest that $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ can be written as

$$G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}') \equiv \hbar\langle\Psi_{N;0}|\big[\widehat{L}^{m-1}\hat\psi_\sigma(\boldsymbol{r}),\hat\psi_\sigma^\dagger(\boldsymbol{r}')\big]_+|\Psi_{N;0}\rangle,\quad m\ge1, \tag{34}$$

where the Liouville super-operator $\widehat{L}\equiv\widehat{L}^1$ is defined as [43]

$$\widehat{L}\hat\phi {:=} \big[\hat\phi,\widehat{H}\big]_-, \tag{35}$$

with $\hat\phi$ any operator in the second-quantization representation. The validity of Eq. (34) is easily verified through substituting the RHS of Eq. (34) in that of Eq. (27) and formally carrying out the infinite sum $\sum_{m=1}^{\infty}(\widehat{L}/z)^{m-1} = \big(I-\widehat{L}/z\big)^{-1}$, thus obtaining

$$\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z) = \hbar\langle\Psi_{N;0}|\Big[\big(zI-\widehat{L}\big)^{-1}\hat\psi_\sigma(\boldsymbol{r}),\hat\psi_\sigma^\dagger(\boldsymbol{r}')\Big]_+|\Psi_{N;0}\rangle, \tag{36}$$

which is the Mori-Zwanzig (Mori 1965, Zwanzig 1961) expression for $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ (see also Fulde (1991)). This result in addition demonstrates *completeness* of the series in Eq. (27) for *all* z. [44]

We note that for $m>2$, the direct application of the expression in Eq. (34), corresponding to the $\widehat{H}$ in Eqs. (1) and (2) leads to extremely complicated expressions. As we shall see in the following subsections, calculation of $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ is greatly facilitated through introduction of auxiliary fields and transposition of the $\widehat{H}$ operators that are implied by $\widehat{L}^{m-1}\hat\psi_\sigma(\boldsymbol{r})$ (in exchange for commutators of $\widehat{H}$ with its adjacent field operators) to the left or right of all other operators; [45] only after this, should the explicit expression for $\widehat{H}$ as presented in Eqs. (1) and (2)

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[42] As we shall discuss later, the set $\{f_{s;\sigma}(\boldsymbol{r})\}$ is *overcomplete*, a fact manifested in the property $\int \mathrm{d}^d r\, f_{s;\sigma}^*(\boldsymbol{r}) f_{s;\sigma}(\boldsymbol{r}) < 1$, for *at least* one s, when $v\not\equiv0$ (see Appendix A).

[43] By definition, $\widehat{L}^0 = I$, the unit operator in the space of $\{\hat\phi\}$, so that $\widehat{L}^0\hat\phi=\hat\phi$.

[44] The result in Eq. (34) is directly deduced by employing those in Eqs. (37) and (38) below; making use of the time-integral representation of $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon\pm i\eta)$ (that is the inverse of that presented in Eq. (E9)), $G_{\sigma;\infty_m}^{(E)}(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (38) is seen to be determined by $\mathrm{d}^{m-1}G_\sigma(\boldsymbol{r}t,\boldsymbol{r}'0)/\mathrm{d}t^{m-1}$ which following the defining expression in Eq. (E7) and the Heisenberg equation of motion (Fetter and Walecka 1971, Eq. (6.29)) (see also Appendix E, and in particular Eq. (E6)) $i\hbar\,\mathrm{d}\hat\psi_\sigma(\boldsymbol{r}t)/\mathrm{d}t = \widehat{L}\hat\psi_\sigma(\boldsymbol{r}t)$, directly results in the expression on the RHS of Eq. (34).

[45] For an *odd* value of m, $\widehat{L}^{m-1}\hat\psi_\sigma(\boldsymbol{r})$ in the expression for $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ (see Eq. (34)) involves an *even* number of $\widehat{H}$, of which $(m-1)/2$ can be transposed to the left and $(m-1)/2$ to the right. This directly gives rise to an expression for $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ in terms of GS correlation functions which *explicitly* satisfies the symmetry requirement (see Appendix B; see also Eq. (178) below) $G_{\sigma;\infty_m}(\boldsymbol{r}',\boldsymbol{r}) \equiv G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$. For an *even* value of m, on the other hand, this possibility cannot be exploited to the full (as the last $\widehat{H}$ must be transposed either to the left or to the right), resulting in an expres-

be employed, followed by a process of *normal ordering* of the field operators, transposing all the creation field operators to the left of the annihilation field operators. We should like to emphasize that neglect of this strategy results in such a vast number of terms that render a reliable calculation of *even* $G_{\sigma;\infty_3}$ prohibitively difficult.

B. The single-particle spectral functions $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$

One can represent $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ as follows:

$$G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}') = \lim_{E\to\infty} G^{(E)}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}') \qquad (37)$$

where

$$G^{(E)}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'):=\int_{-E}^{E} \mathrm{d}\varepsilon\; \varepsilon^{m-1} A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon),\;\; m\ge 1, \quad (38)$$

in which

$$A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon):=\frac{1}{2\pi i}\Big\{\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon-i\eta)-\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon+i\eta)\Big\},\quad \eta\downarrow 0, \quad (39)$$

is the spectral function of the single-particle GF. Our use of $\lim_{E\to\infty}\int_{-E}^{E}\mathrm{d}\varepsilon\,(\dots)$ as implied by Eqs. (37) and (38), rather than simply $\int_{-\infty}^{\infty}\mathrm{d}\varepsilon\,(\dots)$, amounts to a representation of the *distribution* $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ (see text following Eq. (28) above) in terms of a sequence of *functions* $G^{(E)}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ for increasing values of E.

From Eq. (27), making use of Eq. (37) followed by substituting herein the RHS of Eq. (38) for $G^{(E)}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ and exchanging the order of the summation over m with the integration over ε and subsequently employing [46] $\frac{1}{z}\sum_{m=1}^{\infty}(\varepsilon/z)^{m-1}=1/(z-\varepsilon)$ and finally taking the limit $E\to\infty$, we obtain

$$\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)\equiv\int_{-\infty}^{\infty}\mathrm{d}\varepsilon\;\frac{A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)}{z-\varepsilon}, \qquad (40)$$

which is the well-known integral representation of the single-particle GF in terms of its spectral function (for example Nozières 1964); making use of $1/(x\pm i\eta)=\wp(1/x)\mp i\pi\delta(x)$ for $\eta\downarrow 0$ (here $\wp$ stands for the Cauchy 'principal value'), it is readily verified that this representation correctly reproduces the defining expression for $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ in Eq. (39). The fact that the exact $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ is recovered from the representation in Eq. (27), as evidenced by both the result in Eqs. (36) and (40), implies the completeness of this representation which in turn demonstrates the sufficiency in the context of the present work of the asymptotic sequence (see § II.B) $\{1,1/z,\dots\}$, corresponding to $|z|\to\infty$.

Although $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ pertaining to systems whose Hamiltonians have unbounded $(N\pm 1)$-particle spectra is *not* bounded for $m\ge m_0$ (for a uniform and isotropic system, specifically in $d=3$ when $v\equiv v_c$, it can be rigorously shown that $m_0=3$; see § III.I.2), [47] the projection of $G^{(E)}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, which we for simplicity assume not to involve any fundamentally unbounded contributions, on to the single-particle Hilbert space of the problem (see Appendix A) has a bounded limit for $E\to\infty$ for *any* finite value of m (in this context it is useful to consider our discussions in § II.B leading to conditions (A)-(C)). To demonstrate this, we first point out that, from the representation in Eq. (28) one has

$$G^{(E)}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')\equiv\hbar\sum_{\substack{s''\\ |\varepsilon_{s'';\sigma}|<E}}\varepsilon^{m-1}_{s'';\sigma}\,f_{s'';\sigma}(\boldsymbol{r})f^*_{s'';\sigma}(\boldsymbol{r}'). \qquad (41)$$

Multiplying both sides of this expression, from left by $f^*_{s;\sigma}(\boldsymbol{r})$ and from right by $f_{s';\sigma}(\boldsymbol{r}')$, and integrating the resulting expression with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$ we obtain

$$\int \mathrm{d}^d r\,\mathrm{d}^d r'\; f^*_{s;\sigma}(\boldsymbol{r})\,G^{(E)}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')\,f_{s';\sigma}(\boldsymbol{r}') = \hbar\sum_{\substack{s''\\ |\varepsilon_{s'';\sigma}|<E}}\varepsilon^{m-1}_{s'';\sigma}\,\langle f_{s;\sigma}|f_{s'';\sigma}\rangle\,\langle f_{s'';\sigma}|f_{s';\sigma}\rangle. \qquad (42)$$

Let $\{\phi_\varsigma(\boldsymbol{r})\}$ be the complete *orthonormal* set of eigenfunctions of the non-interacting single-particle Hamiltonian (see Eqs. (1) and (2))

$$h_0(\boldsymbol{r}):=\tau(\boldsymbol{r})+u(\boldsymbol{r}); \qquad (43)$$

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sion for $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ which, although *implicitly* symmetric, is *explicitly* highly *asymmetric*. For this reason, evaluation of $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ for *even* values of m is far more complicated than that for *odd* values of m, specifically because it turns out to be extremely cumbersome to make explicit the symmetry of the directly evaluated expression for $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$. The latter task can be simplified by replacing an *explicitly* asymmetric $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ by $\frac{1}{2}[G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')+G_{\sigma;\infty_m}(\boldsymbol{r}',\boldsymbol{r})]$. This has, however, the severe disadvantage of masking the unintentional algebraic errors that may have incurred in the process of evaluating the original expression for $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$. *None* of the results presented in this work is based on such a symmetrization procedure.

[46] Formally, we assume that for a given *finite* E, $|z|>E$. Compare with our statement preceding Eq. (27).

[47] The property that for the mentioned Hamiltonians, $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ is unbounded for $m\ge m_0$, with m_0 a *finite* integer, implies that the point of infinity in the z plane is a singular point of $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$. The results in Eqs. (73) - (75) below suggest that the point of infinity *may* also be a singular point of $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$, which our explicit calculations show indeed to be the case.

we have [48]

$$h_0(\boldsymbol{r})\,\phi_\varsigma(\boldsymbol{r}) = \mathsf{e}_\varsigma\,\phi_\varsigma(\boldsymbol{r}), \qquad (44)$$

where, as implied, $\{\varsigma\}$ fully characterizes the entire set of (single-particle) eigenstates of $h_0(\boldsymbol{r})$. We can therefore express the compound variable s characterizing the Lehmann amplitude $f_{s;\sigma}(\boldsymbol{r})$ as follows [49]

$$s = (\varsigma, \alpha), \qquad (45)$$

where α is the so-called "parameter of degeneracy" (Klein and Prange 1958). [50] In general, we can write

$$f_{s;\sigma}(\boldsymbol{r}) \equiv \phi_\varsigma(\boldsymbol{r}) + \delta f_{s;\sigma}(\boldsymbol{r}), \;\; \text{with} \;\; s = (\varsigma, \alpha), \qquad (46)$$

where

$$\delta f_{s;\sigma}(\boldsymbol{r}) \to 0 \quad \text{for} \quad v \to 0. \qquad (47)$$

Since for increasing values of the magnitude of the single-particle excitation energies $\varepsilon_{s;\sigma}$, interaction effects diminish, the result in Eq. (47) is equally applicable to the cases where $|\varepsilon_{s;\sigma}| \to \infty$. Under either of these two conditions (i.e. $v \to 0$ and/or $|\varepsilon_{s;\sigma}| \to \infty$), which we designate as conditions of 'weak correlation', making use of the orthonormality relation $\langle \phi_\varsigma | \phi_{\varsigma'} \rangle = \delta_{\varsigma,\varsigma'}$, we have

$$\langle f_{s;\sigma} | f_{s';\sigma} \rangle \sim \delta_{s,s'} \equiv \delta_{\varsigma,\varsigma'} \quad (\text{'weak correlation'}), \qquad (48)$$

where in the last equality we have made explicit that under the indicated condition, the 'parameters of degeneracy' α and α', in $s = (\varsigma, \alpha)$ and $s' = (\varsigma', \alpha')$, are irrelevant to the leading order in the interaction. Note that Eq. (48) applies even for $v \not\to 0$ when one or both of the conditions $|\varepsilon_{s;\sigma}| \to \infty$ and $|\varepsilon_{s';\sigma}| \to \infty$ (also identified with 'weak correlation' conditions) are satisfied.

From Eq. (42) for sufficiently 'weak correlation' (see above) we obtain

$$\frac{1}{\hbar} \lim_{E\to\infty} \int \mathrm{d}^d r \mathrm{d}^d r'\; f_{s;\sigma}^*(\boldsymbol{r}) G_{\sigma;\infty_m}^{(E)}(\boldsymbol{r}, \boldsymbol{r}') f_{s';\sigma}(\boldsymbol{r}') \sim \delta_{s,s'}\,\varepsilon_{s;\sigma}^{m-1}, \qquad (49)$$

which is indeed finite for any finite value of m. Since $G_{\sigma;\infty_1}(\boldsymbol{r}, \boldsymbol{r}') = \hbar\delta(\boldsymbol{r} - \boldsymbol{r}')$ (see Eq. (30) above), for $m = 1$, Eq. (49) is seen exactly to reproduce Eq. (48). This establishes the consistency of our above arguments. Making use of Eqs. (38) and (49) we finally obtain

$$\frac{1}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}\varepsilon\; \varepsilon^{m-1}\, \mathsf{A}_{\sigma;s,s'}(\varepsilon) \sim \delta_{s,s'}\,\varepsilon_{s;\sigma}^{m-1} \qquad (\text{'weak correlation'}) \qquad (50)$$

where

$$\mathsf{A}_{\sigma;s,s'}(\varepsilon) := \int \mathrm{d}^d r \mathrm{d}^d r'\; f_{s;\sigma}^*(\boldsymbol{r}) A_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon) f_{s';\sigma}(\boldsymbol{r}'). \qquad (51)$$

Considering uniform and isotropic systems, we have $\{\phi_\varsigma(\boldsymbol{r})\} \equiv \{\Omega^{-1/2} \exp(i\boldsymbol{k}\cdot\boldsymbol{r})\}$ (implying identification of ς with $\boldsymbol{k}$). [51] Under the conditions of 'weak correlation', from Eqs. (46), (47) and (51) we thus obtain

$$\mathsf{A}_{\sigma;s,s'}(\varepsilon) \sim \overline{\mathsf{A}}_{\sigma;\boldsymbol{k},\boldsymbol{k}'}(\varepsilon) \equiv \overline{A}_\sigma(\|\boldsymbol{k}\|; \varepsilon)\,\delta_{\boldsymbol{k},\boldsymbol{k}'}. \qquad (52)$$

From this and Eq. (50) we deduce the following expression

$$\frac{1}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}\varepsilon\; \varepsilon^{m-1}\, \overline{A}_\sigma(\|\boldsymbol{k}\|; \varepsilon) \sim \varepsilon_{\boldsymbol{k};\sigma}^{m-1}. \qquad (53)$$

Here and in Eq. (52), $\overline{A}_\sigma(\|\boldsymbol{k}\|; \varepsilon)$ stands for the Fourier transform with respect to $\boldsymbol{r} - \boldsymbol{r}'$ of $A_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ defined in Eq. (39) above (see § III.I.2). The asymptotic result in Eq. (53) becomes the more accurate (i.e. it applies to cases with smaller values of $|\varepsilon_{\boldsymbol{k};\sigma}|$, or of $\|\boldsymbol{k}\|$) the weaker the strength of the particle-particle interaction. We shall encounter Eq. (53) in § III.E.6 and further discuss its range of applicability.

It is interesting to recall that the assumption with regard to the one-to-one correspondence between $\{\phi_\varsigma(\boldsymbol{r})\}$

[48] Our remarks in footnote 39 apply equally here, that is the 'spectrum' of $h_0(\boldsymbol{r})$ is *not* exhausted by its 'point spectrum', etc.

[49] We note that ς is also a compound variable; consider the case of periodic crystals (i.e. $u(\boldsymbol{r})$ in Eq. (43) is periodic) where $\{\phi_\varsigma(\boldsymbol{r})\}$ are Bloch functions with $\varsigma = (\boldsymbol{k}, \ell)$, $\boldsymbol{k}$ denoting a vector in the first Brillouin zone of the underlying lattice and ℓ a band index.

[50] The designation "parameter of degeneracy", as employed by Klein and Prange (1958), is somewhat misleading. It is true that excited states of many-particle systems are largely degenerate (see footnote 3 above); however, the necessity for the introduction of the "parameter of degeneracy" does *not* arise from degeneracy of these states *per se*, but from the fact that, for *interacting* systems, the distinctive aspects of the $N \pm 1$-particle ground and excited states, in comparison with the N-particle GS, *cannot* be regarded as being associated with properties of one or other single-particle wavefunction. Consequently, characterization of these states in relation to the N-particle GS *cannot* be solely in terms of parameters describing a single-particle wavefunction. This viewpoint is consistent with the fact that although $\{f_{s;\sigma}(\boldsymbol{r})\}$ is complete, that is its constituent elements satisfy the *closure* relation $\sum_s f_{s;\sigma}(\boldsymbol{r}) f_{s;\sigma}^*(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}')$ (see Eq. (30)), we have $\int \mathrm{d}^d r\, f_{s;\sigma}^*(\boldsymbol{r}) f_{s;\sigma}(\boldsymbol{r}) < 1$ for *at least* one s (unless $v \equiv 0$), which in combination with the former result, implies *overcompleteness* of $\{f_{s;\sigma}(\boldsymbol{r})\}$ (see Appendix A).

[51] In choosing $\Omega^{-1/2} \exp(i\boldsymbol{k}\cdot\boldsymbol{r})$, we have employed the 'box' boundary condition, implying our further use of $\Omega\delta_{\boldsymbol{k},\boldsymbol{k}'}/(2\pi)^d$ instead of $\delta(\boldsymbol{k} - \boldsymbol{k}')$.

and $\{f_{s;\sigma}(\boldsymbol{r})\}$, or that between ς and s, which here is used under the provision of 'weak correlation', is that which underlies the *phenomenological* theory of Landau (1957) concerning the *low*-lying single-particle excitations of interacting systems (for example Pines and Nozières (1966)). As we discuss in § III.C, the choice of $\widehat{H}_0$, the 'non-interacting' Hamiltonian, is not entirely arbitrary, as it is necessary that the GS of $\widehat{H}_0$ be *adiabatically connected* with that of $\widehat{H}$ (see Farid (1997a) and the references herein); this aspect is of vital importance in the context of the Fermi-liquid theory. The significance of this requirement is easily illustrated by considering the case where for *some* σ the eigenvalue of the partial number operator $\widehat{N}_\sigma$ corresponding to the GS of $\widehat{H}_0$ is *not* equal to that corresponding to the GS of $\widehat{H}$. In such a case, *no* number-preserving perturbation Hamiltonian is capable of adiabatically transforming the non-interacting GS into the interacting GS. This specific problem can be circumvented by considering (see Eq. (43) above)

$$\widehat{H}_0 = \sum_\sigma \int \mathrm{d}^d r\; \hat{\psi}_\sigma^\dagger(\boldsymbol{r}) h_{0;\sigma}(\boldsymbol{r}) \hat{\psi}_\sigma(\boldsymbol{r}), \tag{54}$$

$$h_{0;\sigma}(\boldsymbol{r}) {:=} h_0(\boldsymbol{r}) + w_\sigma(\boldsymbol{r}), \tag{55}$$

where $w_\sigma(\boldsymbol{r})$ is *some* spin-dependent local potential chosen in such a way that $\{N_\sigma\}$ is common to the GSs of $\widehat{H}_0$ and $\widehat{H}$. In fact, for the class of interacting number densities $\{n_\sigma(\boldsymbol{r}) \| \sigma = -\mathsf{s}, -\mathsf{s}+1, \dots, \mathsf{s}\}$ (see Eq. (163) below), known as 'pure-state non-interacting v-representable' densities, it is possible to choose $\{w_\sigma(\boldsymbol{r})\}$ in such a way that even $\{n_{0;\sigma}(\boldsymbol{r})\}$ is identical with its interacting counterpart $\{n_\sigma(\boldsymbol{r})\}$ (Farid 1997a,b, 1999b); this statement is most naturally described within the framework of the density-functional theory of Hohenberg and Kohn (1964) (for example Dreizler and Gross (1990)).

From the perspectives of the above considerations, it is therefore more advantageous (see Appendix A) to relate the set of Lehmann amplitudes with the complete set of *orthonormal* eigenstates of the following one-particle problem [52]

$$h_{0;\sigma}(\boldsymbol{r})\, \varphi_{\varsigma;\sigma}(\boldsymbol{r}) = \varepsilon_{\varsigma;\sigma}^{(0)}\, \varphi_{\varsigma;\sigma}(\boldsymbol{r}). \tag{56}$$

All our earlier comments concerning the set $\{\varsigma\}$ corresponding to the non-interacting eigenvalue problem in Eq. (44) apply here. It is natural that $w_\sigma(\boldsymbol{r})$ be chosen in such a way that for $v \to 0$ it approaches zero or at most a constant, independent of $\boldsymbol{r}$. Further, since for $|\varepsilon_{\varsigma;\sigma}^{(0)}| \to \infty$, $\tau(\boldsymbol{r})\varphi_{\varsigma;\sigma}(\boldsymbol{r}) \sim \varepsilon_{\varsigma;\sigma}^{(0)}\, \varphi_{\varsigma;\sigma}(\boldsymbol{r})$, which also applies to $\phi_\varsigma(\boldsymbol{r})$ when $|\mathsf{e}_\varsigma| \to \infty$, that is $\tau(\boldsymbol{r})\phi_\varsigma(\boldsymbol{r}) \sim \mathsf{e}_\varsigma \phi_\varsigma(\boldsymbol{r})$, it follows that under the conditions of 'weak correlation', specified in the text following Eq. (48) above, the eigenvalue problem in Eq. (56) is interchangeable with and, for the reason indicated, preferable to that in Eq. (44) (see Appendix A). It follows that Eqs. (48)-(53) retain their validity by choosing the 'non-interacting' problem to be that corresponding to $h_{0;\sigma}(\boldsymbol{r})$ in Eq. (55) (see also footnote 52) rather than that corresponding to $h_0(\boldsymbol{r})$ in Eq. (43).

For completeness, we note that from Eqs. (30) and (38) one has

$$\frac{1}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}\varepsilon\; A_\sigma(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon) = \delta(\boldsymbol{r} - \boldsymbol{r}'), \tag{57}$$

the RHS of which is evidently *in*dependent of the strength of the particle-particle interaction, so that Eq. (57) equally applies to *non*-interacting systems. The result in Eq. (57) is in fact nothing but a statement concerning the *completeness* or *closure* of both $\{f_{s;\sigma}(\boldsymbol{r})\}$ (see Eq. (30)) and $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$ in the single-particle Hilbert space of the system under consideration (see Appendix A). We point out that, under the conditions where Eq. (48) as well as other related expressions apply, one can replace s, s' by ς and ς' respectively. Thus, in contrast with the *exact* case where the non-trivial dependence of $\varepsilon_{s;\sigma}$ on α through $s = (\varsigma, \alpha)$ implies that the single-particle excitation energies are *not* sharply defined but are rather associated with peaks of finite widths in the single-particle spectral functions pertaining to interacting systems, in the cases pertinent to Eqs. (50) and (53), the energies $\varepsilon_{\varsigma,\sigma}$ are sharply defined. Consequently, the latter energies should only be indicative of the *average* locations of well-defined peaks of the single-particle spectral function along the ε axis (see § III.D).

Before closing this Section, we mention that the series in Eq. (27) has an alternative of the form

$$\widetilde{G}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z) = \sum_{m=1}^{\infty} \frac{G_{\sigma;(1/\varepsilon_0)_m}(\boldsymbol{r}, \boldsymbol{r}')}{(z - \varepsilon_0)^m}; \tag{58}$$

here ε_0 is a *real* constant energy, so that for $\mathrm{Im}(z) \neq 0$, the expression in Eq. (58) correctly reproduces the exact reflection property in Eq. (26). As can be readily seen, the expression in Eq. (27) corresponds to the case where $\varepsilon_0 = 0$; we have made this fact explicit by introducing the subscript $(1/\varepsilon_0)_m$ in the coefficient functions on the RHS of Eq. (58). The expression in Eq. (58) can be viewed as an infinite-order AS in terms of the asymptotic sequence $\{1, 1/(z-\varepsilon_0), 1/(z-\varepsilon_0)^2, \dots\}$ appropriate for $|z - \varepsilon_0| \to \infty$.

The relationship between $\{G_{\sigma;\infty_m}\}$ and $\{G_{\sigma;(1/\varepsilon_0)_m}\}$ is direct and can be revealed as follows. By writing the denominator of the integrand on the RHS of Eq. (40) as $(z - \varepsilon_0)[1 - (\varepsilon - \varepsilon_0)/(z - \varepsilon_0)]$, making use of the geometric series for $1/[1 - (\varepsilon - \varepsilon_0)/(z - \varepsilon_0)]$ and subsequently employing the binomial expansion

[52] The left-hand side of Eq. (56) may even accommodate a *non-local* contribution, of the form $\int \mathrm{d}^d r'\; \Upsilon(\boldsymbol{r}, \boldsymbol{r}')\varphi_{\varsigma;\sigma}(\boldsymbol{r}')$, where $\Upsilon_\sigma(\boldsymbol{r}, \boldsymbol{r}')$ may be chosen to be $\Sigma_{\sigma;\infty_0}^{\sharp}(\boldsymbol{r}, \boldsymbol{r}')$, introduced in Eq. (72) below.

$$(\varepsilon-\varepsilon_0)^m = \sum_{j=0}^{m} \binom{m}{j} (-\varepsilon_0)^{m-j} \varepsilon^j,$$

from Eq. (58) we immediately obtain the following results: [53]

$$G_{\sigma;(1/\varepsilon_0)_m}(\boldsymbol{r},\boldsymbol{r}') \equiv \int \mathrm{d}\varepsilon\; (\varepsilon-\varepsilon_0)^{m-1}\, A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$$
$$= \sum_{j=0}^{m-1} \binom{m-1}{j} (-\varepsilon_0)^{m-j-1}\, G_{\sigma;\infty_{j+1}}(\boldsymbol{r},\boldsymbol{r}'); \qquad (59)$$

by restricting the ε integral in Eq. (59) to the interval $(-E,E)$, we obtain what we denote by $G^{(E)}_{\sigma;(1/\varepsilon_0)_m}(\boldsymbol{r},\boldsymbol{r}')$ in terms of $\{G^{(E)}_{\sigma;\infty_j}(\boldsymbol{r},\boldsymbol{r}')\}$ defined in Eqs. (38) and (41). The first equality in Eq. (59) implies that $\{G_{\sigma;(1/\varepsilon_0)_m}(\boldsymbol{r},\boldsymbol{r}')\}$ are the *central* ε moments of the single-particle spectral function with respect to ε_0, while the second equality makes explicit the association between $G_{\sigma;(1/\varepsilon_0)_m}$ and the entire set $\{G_{\sigma;\infty_1},\dots,G_{\sigma;\infty_m}\}$.

Making use of

$$\varepsilon^{m-1} \equiv (\varepsilon-\varepsilon_0+\varepsilon_0)^{m-1}$$
$$\equiv \sum_{j=0}^{m-1} \binom{m-1}{j} (\varepsilon_0)^{m-j-1} (\varepsilon-\varepsilon_0)^j$$

in the integral on the RHS of Eq. (38) (identifying herein E with ∞) and comparing the result with the first expression on the RHS of Eq. (59), we readily obtain the inverse of the second expression on the RHS of Eq. (59), namely

$$G_{\sigma;\infty_m} = \sum_{j=0}^{m-1} \binom{m-1}{j} (\varepsilon_0)^{m-j-1}\, G_{\sigma;(1/\varepsilon_0)_{j+1}}. \qquad (60)$$

Note the change of $(-\varepsilon_0)$ in the RHS of Eq. (59) into (ε_0) on the RHS of Eq. (60).

C. Specific details

In what follows we deal with *formal* truncated AS for $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ and $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ for arbitrary interaction potentials v and spatial dimensions d, *without* considering whether the coefficients in these series are bounded or not (*cf.* a_j^{b} and a_j^{u} introduced in § II.B). Later, we shall in detail consider the issues related to the existence of the mentioned coefficients. It is important to realize that truncation of the infinite series for $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ in Eq. (27) (or Eq. (58)), as well as that for $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ (see Eq. (72) below), results in functions (which for the moment we assume to be well defined) that are analytic *everywhere* in the complex z plane except at the origin (or at $z=\varepsilon_0$), where they possess a multiple *pole* whose order depends on the number of terms incorporated in the pertinent finite-order AS. Although these series are appropriate for the region $|z|\to\infty$, the latter observation is relevant in that it shows that, in contrast with the exact functions $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ and $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$, the corresponding (finite-order) AS are single valued. [54] Since the coefficients in these formal finite-order series are real valued (see Appendix B; see also Eq. (178) below), for cases where $\mathrm{Im}(z)=0$, these series are consequently also real-valued. In § III.I we show that any *formal* finite-order AS for $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$, as $|z|\to\infty$, reduces to a *formal* AS for $\mathrm{Re}[\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)]$, when $z\to\varepsilon\pm i\eta$, with $\eta\downarrow 0$ (*cf.* Eq. (65) below); in this Section we also show how, from the latter, the large-$|\varepsilon|$ AS for $\mathrm{Im}[\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)]$ can be deduced and derive the *explicit* expression for this series up to terms decreasing not more rapidly than $1/\varepsilon^2$. Making use of this as well as some other results that we obtain later in this paper, in § III.I.2 we calculate the explicit AS (up to and including the second leading term for the cases corresponding to bounded and short-range interaction functions and the third leading term for the cases corresponding to $d=3$ and $v\equiv v_c$) for the Fourier transform of the single-particle spectral function pertaining to a uniform and isotropic system of fermions.

In view of our explicit calculations in the present paper, we restrict ourselves to considering the four leading terms of the infinite series in Eq. (27) and write

$$\widetilde{G}_\sigma(z) \sim \frac{\hbar I}{z} + \frac{G_{\sigma;\infty_2}}{z^2} + \frac{G_{\sigma;\infty_3}}{z^3} + \frac{G_{\sigma;\infty_4}}{z^4}, \quad |z|\to\infty, \qquad (61)$$

where we have employed a representation-free notation and used the result in Eq. (30). [55] With reference to our considerations in § II.B, we emphasize that the series in Eq. (61) is at this stage merely a formal device, since in general the coefficients $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, $m=2,3,4$, do *not* satisfy the equivalents of the criteria (A)-(C) in § II.B (which concern $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$) for $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$.

Before entering into details, we mention that, whereas $\widetilde{G}_\sigma(z)$ corresponding to $\widehat{H}$ is well-specified, the freedom in the choice of the non-interacting Hamiltonian $\widehat{H}_0$ implies that this is not the case for $\widetilde{G}_{0;\sigma}(z)$. Traditionally, the SE operator $\widetilde{\Sigma}_\sigma(z)$ is defined with respect to the

[53] Here we define $(0)^{m-j}=\delta_{m,j}$.

[54] We leave aside the fact that $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ is a *bounded* function (almost everywhere in the $\boldsymbol{r}$ and $\boldsymbol{r}'$ space) over the entire z plane, including $z=0$ (or $z=\varepsilon_0$).

[55] Recall that for the unit operator I in the single-particle Hilbert space we have $\langle\boldsymbol{r}|I|\boldsymbol{r}'\rangle=\delta(\boldsymbol{r}-\boldsymbol{r}')$ (see text following Eq. (81) below).

$\widetilde{G}_{0;\sigma}(z)$ pertaining to the truly non-interacting Hamiltonian, that is $\widehat{H}_0{:=}\widehat{T}+\widehat{U}$. However, as $\{\widetilde{G}_{0;\sigma}(z)\}$ is defined in terms of the GS of $\widehat{H}_0$, it is possible that the $\{N_\sigma\}$ corresponding to this GS is different from that corresponding to the GS of $\widehat{H}$, in which case $\widetilde{G}_{0;\sigma}(z)$ and $\widetilde{G}_\sigma(z)$ *cannot* be directly related to one another through $\widetilde{\Sigma}_\sigma(z)$. To circumvent this problem, in this work we assume $\widehat{H}_0$ to be defined as in Eq. (54) in terms of $h_{0;\sigma}(\boldsymbol{r})$ in Eq. (55).

In the light of the above, in the following we denote the SE operator corresponding to $\widehat{H}'{:=}\widehat{H}-\widehat{H}_0$, with $\widehat{H}_0$ as defined in Eq. (54), by $\widetilde{\Sigma}^\sharp_\sigma(z)$, to be distinguished from $\widetilde{\Sigma}_\sigma(z)$, for which we have

$$\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)\equiv\widetilde{\Sigma}^\sharp_\sigma(\boldsymbol{r},\boldsymbol{r}';z)+\frac{1}{\hbar}w_\sigma(\boldsymbol{r})\delta(\boldsymbol{r}-\boldsymbol{r}'). \quad (62)$$

From the Dyson equation

$$\widetilde{G}_\sigma(z)=\widetilde{G}_{0;\sigma}(z)+\widetilde{G}_{0;\sigma}(z)\widetilde{\Sigma}^\sharp_\sigma(z)\widetilde{G}_\sigma(z) \quad (63)$$

we have (use of $\widetilde{\Sigma}^\sharp_\sigma(z)$ in Eq. (63) implies that $\widetilde{G}_{0;\sigma}(z)$ herein pertains to the single-particle Hamiltonian $h_{0;\sigma}(\boldsymbol{r})$ in Eq. (55), to be distinguished from $h_0(\boldsymbol{r})$ in Eq. (43))

$$\widetilde{\Sigma}^\sharp_\sigma(z)=\widetilde{G}^{-1}_{0;\sigma}(z)-\widetilde{G}^{-1}_\sigma(z). \quad (64)$$

Above $\widetilde{\Sigma}_\sigma(z)$ and $\widetilde{\Sigma}^\sharp_\sigma(z)$ stand for the analytic continuations into the physical Riemann sheet of the SE operators $\Sigma_\sigma(\varepsilon)$ and $\Sigma^\sharp_\sigma(\varepsilon)$ respectively; the latter are recovered from the former according to (*cf.* Eq. (25) above)

$$\Sigma_\sigma(\varepsilon)=\lim_{\eta\downarrow 0}\widetilde{\Sigma}_\sigma(\varepsilon\pm i\eta),\quad \varepsilon\gtrless\mu, \quad (65)$$

$$\Sigma^\sharp_\sigma(\varepsilon)=\lim_{\eta\downarrow 0}\widetilde{\Sigma}^\sharp_\sigma(\varepsilon\pm i\eta),\quad \varepsilon\gtrless\mu. \quad (66)$$

We point out that, similar to $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$, $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ possesses the reflection property (see Eq. (26) above)

$$\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z^*)\equiv\widetilde{\Sigma}^*_\sigma(\boldsymbol{r},\boldsymbol{r}';z)\quad\text{when}\quad \mathrm{Im}(z)\neq 0. \quad (67)$$

The expression in Eq. (64) serves to provide us with the AS of $\widetilde{\Sigma}_\sigma(z)$ for $|z|\to\infty$ from those of $\widetilde{G}_{0;\sigma}(z)$ and $\widetilde{G}_\sigma(z)$. This is achieved through employing the following, which amounts to a generalization of a theorem from the calculus of asymptotic expansions (Copson 1965, pp. 8 and 9): [56] Let $\tilde{f}(z)$ possess the following AS with respect to the asymptotic sequence $\{1/z^m \| m=0,1,2,\dots\}$,

$$\tilde{f}(z)\sim\frac{f_1}{z}+\frac{f_2}{z^2}+\dots,\quad |z|\to\infty. \quad (68)$$

[56] The generalization concerns extending a result applicable to *scalar functions* to *operators*, taking due account of the proper ordering of the operators.

Then, provided $\det(f_1)\neq 0$, one has

$$\tilde{f}^{-1}(z)\sim z f_1^{-1}+f_0'+\frac{f_1'}{z}+\frac{f_2'}{z^2}+\dots,\quad |z|\to\infty, \quad (69)$$

where

$$\begin{aligned} f_0' &\equiv -f_1^{-1}f_2f_1^{-1},\\ f_1' &\equiv f_1^{-1}\big(f_2f_1^{-1}f_2-f_3\big)f_1^{-1},\\ f_2' &\equiv -f_1^{-1}\big(f_2f_1^{-1}f_2f_1^{-1}f_2-f_2f_1^{-1}f_3\\ &\qquad -f_3f_1^{-1}f_2+f_4\big)f_1^{-1}. \end{aligned} \quad (70)$$

From the AS in Eq. (27) (or Eq. (61)) we thus obtain

$$\begin{aligned}\widetilde{G}^{-1}_\sigma(z) &\sim \frac{zI}{\hbar}-\frac{G_{\sigma;\infty_2}}{\hbar^2}+\frac{G^2_{\sigma;\infty_2}-\hbar G_{\sigma;\infty_3}}{\hbar^3 z}\\ &-\frac{G^3_{\sigma;\infty_2}-\hbar G_{\sigma;\infty_2}G_{\sigma;\infty_3}-\hbar G_{\sigma;\infty_3}G_{\sigma;\infty_2}+\hbar^2 G_{\sigma;\infty_4}}{\hbar^4 z^2}\\ &+\dots. \end{aligned} \quad (71)$$

The same expression applies to $\widetilde{G}^{-1}_{0;\sigma}(z)$, with the operators $G_{\sigma;\infty_p}$, $p=2,3,4,\dots$, on the RHS replaced by $G_{0;\sigma;\infty_p}$. Making use of these results and Eq. (64), we readily obtain

$$\widetilde{\Sigma}^\sharp_\sigma(z)\sim\Sigma^\sharp_{\sigma;\infty_0}+\frac{\Sigma_{\sigma;\infty_1}}{z}+\frac{\Sigma_{\sigma;\infty_2}}{z^2}+\dots,\quad |z|\to\infty, \quad (72)$$

where

$$\Sigma^\sharp_{\sigma;\infty_0}\equiv\frac{-1}{\hbar^2}\big\{G_{0;\sigma;\infty_2}-G_{\sigma;\infty_2}\big\}, \quad (73)$$

$$\begin{aligned}\Sigma_{\sigma;\infty_1} &\equiv \frac{1}{\hbar^3}\big\{G^2_{0;\sigma;\infty_2}-G^2_{\sigma;\infty_2}\big\}\\ &-\frac{1}{\hbar^2}\big\{G_{0;\sigma;\infty_3}-G_{\sigma;\infty_3}\big\}\end{aligned} \quad (74)$$

$$\begin{aligned}\Sigma_{\sigma;\infty_2} &\equiv \frac{-1}{\hbar^4}\big\{G^3_{0;\sigma;\infty_2}-G^3_{\sigma;\infty_2}\big\}\\ &+\frac{1}{\hbar^3}\big\{G_{0;\sigma;\infty_2}G_{0;\sigma;\infty_3}-G_{\sigma;\infty_2}G_{\sigma;\infty_3}\\ &\qquad +G_{0;\sigma;\infty_3}G_{0;\sigma;\infty_2}-G_{\sigma;\infty_3}G_{\sigma;\infty_2}\big\}\\ &-\frac{1}{\hbar^2}\big\{G_{0;\sigma;\infty_4}-G_{\sigma;\infty_4}\big\}.\end{aligned} \quad (75)$$

These results clarify our restriction to the finite series in Eq. (61). Note that the *independence* from z of the difference between $\widetilde{\Sigma}^\sharp_\sigma(z)$ and $\widetilde{\Sigma}_\sigma(z)$ (see Eq. (62) above) implies that *only* the leading asymptotic term of these SEs are different; explicitly,

$$\begin{aligned}\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}') &= \Sigma^\sharp_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')+\frac{1}{\hbar}w_\sigma(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}'),\\ \Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}') &\equiv \Sigma^\sharp_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'),\quad m\geq 1.\end{aligned} \quad (76)$$

This aspect, which clarifies our notation in Eq. (72), implies that in the expressions for $\Sigma_{\sigma;\infty_m}$, $m=1,2$, in

Eqs. (74) and (75), the dependence upon w_σ of $G^2_{0;\sigma;\infty_2}$ must cancel that of $G_{0;\sigma;\infty_3}$ and similarly for $G^3_{0;\sigma;\infty_2}$ and $G_{0;\sigma;\infty_4}$, etc. (note that, since the Hamiltonian $\widehat{H}$ is independent of w_σ, $G_{\sigma;\infty_m}$ and its various powers are naturally independent of w_σ); this we shall explicitly demonstrate in the following. On the basis of these considerations, the results in Eqs. (74) and (75) reduce into the following

$$\Sigma_{\sigma;\infty_1} = \frac{1}{\hbar^3}\big\{\hbar G_{\sigma;\infty_3} - G^2_{\sigma;\infty_2}\big\}, \qquad (77)$$

$$\Sigma_{\sigma;\infty_2} = \frac{1}{\hbar^4}\big\{\hbar^2 G_{\sigma;\infty_4} - \hbar G_{\sigma;\infty_2} G_{\sigma;\infty_3} - \hbar G_{\sigma;\infty_3} G_{\sigma;\infty_2} + G^3_{\sigma;\infty_2}\big\}. \qquad (78)$$

With reference to the alternative series expansion in Eq. (58), we note that the SE operator similarly admits of the following series (*cf.* Eq. (72))

$$\Sigma^\sharp_\sigma(z) \sim \Sigma^\sharp_{\sigma;(1/\varepsilon_0)_0} + \frac{\Sigma_{\sigma;(1/\varepsilon_0)_1}}{z-\varepsilon_0} + \frac{\Sigma_{\sigma;(1/\varepsilon_0)_2}}{(z-\varepsilon_0)^2} + \dots, \quad |z-\varepsilon_0| \to \infty, \qquad (79)$$

where the coefficient operators $\Sigma^\sharp_{\sigma;(1/\varepsilon_0)_0}$, $\Sigma_{\sigma;(1/\varepsilon_0)_1}$ and $\Sigma_{\sigma;(1/\varepsilon_0)_2}$ are obtained from the expressions in Eqs. (73), (74) and (75) in which $G_{0;\sigma;\infty_m}$ and $G_{\sigma;\infty_m}$ are replaced by $G_{0;\sigma;(1/\varepsilon_0)_m}$ and $G_{\sigma;(1/\varepsilon_0)_m}$ respectively. The latter operators are obtained from the former ones through the second expression on the RHS of Eq. (59). In this way one obtains the coefficients in the series in Eq. (79) in terms of those in Eq. (72) which we explicitly consider in this work. One can alternatively obtain the explicit expressions for $\{\Sigma_{\sigma;(1/\varepsilon_0)_m}\}$ in terms of $\{\Sigma_{\sigma;\infty_m}\}$ through employing the RHS of

$$\frac{1}{z^m} \equiv \frac{1}{(z-\varepsilon_0)^m} \sum_{j=0}^{\infty} (-1)^j \Big[\sum_{j'=1}^{m} \binom{m}{j'} \Big(\frac{\varepsilon_0}{z-\varepsilon_0}\Big)^{j'}\Big]^j \qquad (80)$$

in that of Eq. (72) and, in view of the expression on the RHS of Eq. (79), identifying in the resulting expression the coefficient of $1/(z-\varepsilon_0)^m$ with $\Sigma_{\sigma;(1/\varepsilon_0)_m}$. In this way one readily obtains

$$\begin{aligned}
&\Sigma^\sharp_{\sigma;(1/\varepsilon_0)_0} \equiv \Sigma^\sharp_{\sigma;\infty_0},\\
&\Sigma_{\sigma;(1/\varepsilon_0)_1} \equiv \Sigma_{\sigma;\infty_1},\\
&\Sigma_{\sigma;(1/\varepsilon_0)_2} \equiv \Sigma_{\sigma;\infty_2} - \varepsilon_0\, \Sigma_{\sigma;\infty_1}.
\end{aligned} \qquad (81)$$

In the following Sections, we explicitly evaluate $G_{\sigma;\infty_m}$, with $m = 2, 3, \dots$, and $\Sigma_{\sigma;\infty_m}$, with $m = 0, 1, \dots$, in the coordinate representation, where we have to do with $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}') \equiv \langle \boldsymbol{r}|G_{\sigma;\infty_m}|\boldsymbol{r}'\rangle$ and $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}') \equiv \langle \boldsymbol{r}|\Sigma_{\sigma;\infty_m}|\boldsymbol{r}'\rangle$. Here $|\boldsymbol{r}\rangle$ and $|\boldsymbol{r}'\rangle$ stand for the eigenstates of the $\hat{\boldsymbol{r}}$ operator, corresponding to eigenvalues $\boldsymbol{r}$ and $\boldsymbol{r}'$ respectively, which satisfy the normalization condition $\langle \boldsymbol{r}|\boldsymbol{r}'\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}')$. Consequently, for the lth power of an operator O (representing $G_{\sigma;\infty_m}$), making use of the 'decomposition' of the unit operator in the single-particle Hilbert space, namely

$$I = \int \mathrm{d}^d r\; |\boldsymbol{r}\rangle\langle \boldsymbol{r}|, \qquad (82)$$

one has

$$\begin{aligned}
\langle \boldsymbol{r}|\mathsf{O}^2|\boldsymbol{r}'\rangle &= \int \mathrm{d}^d r_1\; \langle \boldsymbol{r}|\mathsf{O}|\boldsymbol{r}_1\rangle\langle \boldsymbol{r}_1|\mathsf{O}|\boldsymbol{r}'\rangle,\\
\langle \boldsymbol{r}|\mathsf{O}^l|\boldsymbol{r}'\rangle &= \int \mathrm{d}^d r_1\; \dots \mathrm{d}^d r_{l-1}\\
&\quad\times \langle \boldsymbol{r}|\mathsf{O}|\boldsymbol{r}_1\rangle\langle \boldsymbol{r}_1|\mathsf{O}|\boldsymbol{r}_2\rangle \dots \langle \boldsymbol{r}_{l-1}|\mathsf{O}|\boldsymbol{r}'\rangle, \quad l > 2.
\end{aligned} \qquad (83)$$

D. On the quasi-particle energies and wavefunctions

It is well known that the 'quasi-particle' wavefunctions $\{\psi_{\varsigma;\sigma}(\boldsymbol{r};\varepsilon)\}$ and energies $\{\varepsilon_{\varsigma;\sigma}\}$ are obtained through solving the following two equations (see Eqs. (44) and (56) above)

$$h_{0;\sigma}(\boldsymbol{r})\,\psi_{\varsigma;\sigma}(\boldsymbol{r};\varepsilon) + \hbar \int \mathrm{d}^d r'\; \Sigma^\sharp_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)\,\psi_{\varsigma;\sigma}(\boldsymbol{r}';\varepsilon) = \mathcal{E}_{\varsigma;\sigma}(\varepsilon)\,\psi_{\varsigma;\sigma}(\boldsymbol{r};\varepsilon), \qquad (84)$$

$$\mathcal{E}_{\varsigma;\sigma}(\varepsilon_{\varsigma;\sigma}) = \varepsilon_{\varsigma;\sigma}. \qquad (85)$$

For a given $(\varsigma;\sigma)$, however, Eq. (85) may *not* have a solution (Farid 1999a,c). In cases where Eq. (85) does have a solution, this may *not* be a *regular* solution, characterized by the property of at least once continuous differentiability of $\mathcal{E}_{\varsigma;\sigma}(\varepsilon)$ with respect to ε in a neighbourhood of the solution; such non-regular solution is exemplified by the Fermi energy ε_F of metallic states of one-dimensional interacting systems (generically described by the one-dimensional Luttinger (1963) model (Mattis and Lieb 1965) (for a review see Voit (1994))) when momentum (with which ς in our present notation should be identified) is set equal to one of the two Fermi momenta. [57] Furthermore, by the assumption of stability of the GS of the system under consideration, and the *completeness* of the single-particle eigenfunctions $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$ of $h_{0;\sigma}(\boldsymbol{r})$ whose indices $\{\varsigma\}$ are inherited by the set of

[57] As we have emphasized in (Farid 1999a,c), the possible solutions of Eqs. (84) and (85) may *not* correspond to the Landau quasi-particles (whence our above use of the quotation marks in denoting quasi-particles) for, even though such solutions correspond to single-particle excitations in the system, these excitations may *not* be capable of being described (not even asymptotically) in such terms as are specific to single particles, characterized by a 'smooth' energy dispersion (see Appendix A). Metallic interacting systems whose lowest-lying single-particle excitations can be described as such, constitute the Fermi-liquid "universality" class.

eigenfunctions $\{\psi_{\varsigma;\sigma}(\boldsymbol{r};\varepsilon)\}$ in Eq. (84), [58] for a given $(\varsigma;\sigma)$, Eq. (85) *cannot* possess multiple solutions, for such solutions would imply incompleteness [59] of $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$ as regards the Hilbert space of the single-particle excitations of the interacting system, spanned by the overcomplete set of the Lehmann amplitudes $\{f_{s;\sigma}(\boldsymbol{r})\}$ (see Appendix A).

With reference to our discussions in § III.B concerning the distinction between the single-particle orbitals $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$ and the Lehmann amplitudes $\{f_{s;\sigma}(\boldsymbol{r})\}$, and specifically concerning that between indices s and ς (see Eq. (45) above), we point out that *the possibility of non-existence of solutions to Eq. (85) is directly related to the latter distinction.* To clarify this statement, it is important to recall that $\Sigma_\sigma(\varepsilon)$ is *not* Hermitian for arbitrary values of ε. This implies that $\mathcal{E}_{\varsigma;\sigma}(\varepsilon) \equiv \lim_{\eta\downarrow 0} \widetilde{\mathcal{E}}_{\varsigma;\sigma}(\varepsilon \pm i\eta)$, $\varepsilon \gtrless \mu$ (*cf.* Eq. (65) above) is in general complex valued so that, unless $\mathrm{Im}[\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)] \equiv 0$ at $\varepsilon = \varepsilon_0$, because Eq. (85) is satisfied by $\varepsilon = \varepsilon_0$, ε_0 must also be complex valued. Owing to the reflection property in Eq. (67), such a complex-valued solution would imply satisfaction of Eq. (85) also at $\varepsilon = \varepsilon_0^*$. This possibility is ruled out by the assumption with regard to the stability of the (non-degenerate) N-particle GS of the system under consideration. We note in passing that the stability of the GS implies $\mathrm{Im}[\mathcal{E}_{\varsigma;\sigma}(\varepsilon)] \lesseqgtr 0$ for $\varepsilon \gtrless \mu$, $\forall \varsigma, \sigma$ (Luttinger 1961, in particular Eqs. (38), (49) and (50)). Given the fact that for extended systems, $\mathrm{Im}[\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)]$ is a function of ε with unbounded support (see § III.I.2), we observe that from among the innumerably many single-particle excitations (see § III.B), Eq. (85) *may* in principle possess as few as *two* solutions [60] which, as we have just indicated, must be real valued; complex-valued single-particle excitation energies, with the finite imaginary parts corresponding to the finite life-times of the associated single-particle excitations, can be deduced from a pair of equations similar to those in Eqs. (84) and (85) corresponding to the analytic continuation of $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ into *non*-physical Riemann sheets (for details see Farid (1999a,c)). The *overcompleteness* of $\{f_{s;\sigma}(\boldsymbol{r})\}$, which is related to $s = (\varsigma, \alpha)$ (see Eq. (45) above and the associated text in § III.B), on the one hand, and the characterization of the eigenfunctions of Eq. (84) by ς, on the other hand, [61] makes explicit that the role of the "parameter of degeneracy" α (see footnote 50) is in a way taken over by the continuous energy parameter ε in Eq. (84) in combination with the general non-Hermiticity of $\Sigma_\sigma(\varepsilon)$; substituting (ς, α) for s in $\varepsilon_{s;\sigma}$ as defined in Eq. (19), we observe that by the very token that for any given ς (which is capable of characterizing *any* single-particle excitation of the system described by $\widehat{H}_0$ (see Eqs. (54) and (55) above)) there exists a continuous manifold of associated single-particle excitations of the *interacting* system corresponding to the continuous variable α, Eqs. (84) and (85) *must not* be capable of exhausting the spectrum of the single-particle excitations of the interacting system in the form of *isolated* real-valued solutions. [62] Conversely, in cases where, for a given ς, Eqs. (84) and (85) yield a real-valued solution, the 'parameter of degeneracy' must be 'quenched'; the range of variations in α in the neighbourhoods of its 'quenched' values depends on the nature of the associated solutions (i.e. on whether these are isolated, regular or accumulation points).

The significance of the large-$|\varepsilon|$ AS of $\widetilde{\Sigma}_\sigma^\sharp(z)$ in Eq. (72) is made explicit through substituting this series for $\Sigma_\sigma^\sharp(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (*cf.* Eq. (66) above) in Eq. (84). We consider such substitution in the following Section where we explicitly deal with a uniform system in its uniform and isotropic GS. In § III.E.6 we discuss the consequences of neglecting the imaginary part of $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ by a *finite-order* AS for this function. [63] Therefore, suffice it to say

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[58] It is here that the importance of the hypothesis concerning the *adiabatic connection* (see Farid (1997a,b)) between the N-particle GSs of $\widehat{H}_0$ and $\widehat{H}$ becomes most clearly manifest. See § III.C where we briefly elaborate on the significance of $\Sigma_\sigma^\sharp(\varepsilon)$ in comparison with $\Sigma_\sigma(\varepsilon)$.

[59] For the precise definition of *completeness* of normed spaces, and of Cauchy sequences, see Kreyszig (1978) and Debnath and Mikusiński (1990).

[60] Previously (Farid 1999c) we have shown that in general there exist appropriate ς for which $\mathcal{E}_{\varsigma;\sigma}(\mu_{N;\sigma}^{\mp}) = \mu_{N;\sigma}^{\mp}$, where $\mu_{N;\sigma}^{\mp}$ are defined in Eq. (23) above. In (extended) *metallic* systems, $\mu_{N;\sigma}^{-} \equiv \varepsilon_F$, the Fermi energy of the interacting system. In general $\mu_{N;\sigma}^{-} < \mu < \mu_{N;\sigma}^{+}$ (see Eq. (22) above), where μ stands for the 'chemical potential'. In the latter systems, $\mu_{N;\sigma}^{+} - \mu_{N;\sigma}^{-}$ is infinitesimally small (proportional to $1/N^\alpha$ with $\alpha > 0$) so that, by the constancy of μ with respect to $\{\sigma\}$, $\mu_{N;\sigma}^{\pm}$ must be up to an infinitesimal correction *independent* of $\{\sigma\}$. The validity of this statement at finite temperatures is ascribed to the condition of thermodynamic equilibrium between particles, irrespective of their spin index. For completeness, we mention that for *all* $\varepsilon \in [\mu_{N;\sigma}^{-}, \mu_{N;\sigma}^{+}]$ we have the *exact* result $\mathrm{Im}[\mathcal{E}_{\varsigma;\sigma}(\varepsilon)] \equiv 0$ (see Galitskii and Migdal 1958, and Luttinger 1960, equations (6) and (94)).

[61] The eigenfunctions $\{\psi_{\varsigma;\sigma}(\boldsymbol{r};\varepsilon)\}$, with $\psi_{\varsigma;\sigma}(\boldsymbol{r};\varepsilon) \equiv \lim_{\eta\downarrow 0} \widetilde{\psi}(\boldsymbol{r};\varepsilon \pm i\eta)$, $\varepsilon \gtrless \mu$, do *not* form an orthonormal set, but a *bi-orthonormal* set in combination with $\{\psi'_{\varsigma;\sigma}(\boldsymbol{r};\varepsilon)\}$ (Morse and Feshbach 1953, pp. 884-886, Layzer 1963), where $\psi'_{\varsigma;\sigma}(\boldsymbol{r};\varepsilon) := \lim_{\eta\downarrow 0} \tilde{\psi}_{\varsigma;\sigma}(\boldsymbol{r};\varepsilon \mp i\eta)$ for $\varepsilon \gtrless \mu$ (Farid 1999a,c) (*cf.* Eq. (66) above and notice $\mp$ as compared with $\pm$).

[62] This aspect holds true also for finite systems.

[63] We point out that the complex-valuedness of the *regularized* $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ for $m \geq 2$ (see Eq. (110) below), originates from the *infinite* partial summation of unbounded terms in the full large-$|\varepsilon|$ AS for $\Sigma_\sigma^\sharp(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$. We further point out that, *in principle*, it is possible explicitly to take into account

for the moment that, although such a neglect by a finite-order series gives rise to real-valued solutions to Eq. (85), such solutions have direct physical significance through their relevance to the ε-moments integrals of the single-particle spectral function (see § III.B). Further, as we discuss in § III.E.6, the contributions of the latter real-valued solutions to the single-particle spectral function, which show up as poles, can be broadened in a controlled fashion in anticipation of the condensation of these poles into branch cuts of $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ in the limit where the complete infinite AS of this function is taken into account. Note in passing that Eqs. (72) and (76) (see also Eq. (173) below) clearly show the approach of the equation in Eq. (84) to the *exact* Hartree-Fock equation [64] for $|\varepsilon| \to \infty$ (see § I.B).

E. A simple example and some discussions

Below we consider some quantitative aspects associated with finite-order large-$|\varepsilon|$ AS for $\Sigma_\sigma(\varepsilon)$. To this end, we specifically deal with a system of fermions in a uniform positively-charged background. For simplicity, we deal solely with the homogeneous and isotropic GS of this system.

1. The Hamiltonian and some conventions

The system with which we deal is described by the following Hamiltonian (for example Fetter and Walecka (1971, p. 25)):

$$\widehat{H} = \sum_{\sigma'} \sum_{\boldsymbol{k}'} \frac{\hbar^2 k'^2}{2m_e}\, \hat{\mathsf{a}}^\dagger_{\boldsymbol{k}';\sigma'} \hat{\mathsf{a}}_{\boldsymbol{k}';\sigma'} + \frac{1}{2\Omega} \sum_{\sigma_1',\sigma_2'} \sideset{}{'}\sum_{\boldsymbol{k}',\boldsymbol{p}',\boldsymbol{q}'} \bar{v}(q')\, \hat{\mathsf{a}}^\dagger_{\boldsymbol{k}'+\boldsymbol{q}';\sigma_1'} \hat{\mathsf{a}}^\dagger_{\boldsymbol{p}'-\boldsymbol{q}';\sigma_2'} \hat{\mathsf{a}}_{\boldsymbol{p}';\sigma_2'} \hat{\mathsf{a}}_{\boldsymbol{k}';\sigma_1'}, \tag{86}$$

where the prime over $\sum_{\boldsymbol{q}'}'$ implies that the contribution corresponding to $\boldsymbol{q}' = \boldsymbol{0}$ must be excluded. In Eq. (86), $\bar{v}(q')$, with $q' {:=} \|\boldsymbol{q}'\|$, stands for the Fourier transform of the particle-particle interaction function $v(\boldsymbol{r}-\boldsymbol{r}')$; in what follows, we write

$$v(\boldsymbol{r}-\boldsymbol{r}') = g\, w(\boldsymbol{r}-\boldsymbol{r}'), \tag{87}$$

where g stands for the coupling constant of interaction and $w(\boldsymbol{r}-\boldsymbol{r}')$ depends on $\|\boldsymbol{r}-\boldsymbol{r}'\|$; in the case of $v \equiv v_c$ in $d=3$, we have (see Eq. (13) and text following Eq. (15) above)

$$g_c = \frac{e^2}{4\pi\epsilon_0}, \quad \bar{w}_c(q) = \frac{4\pi}{q^2+\kappa^2}, \quad \kappa \downarrow 0, \tag{88}$$

where, owing to the exclusion of $\boldsymbol{q}' = \boldsymbol{0}$ form the $\boldsymbol{q}'$-sum on the RHS of Eq. (86), it is permitted to identify κ with zero without any further consequence. With reference to our considerations in § II.A, we further point out that, in dealing with the case corresponding to $v = v_c$ in $d = 3$, the RHS of Eq. (86) has to be supplemented by $2\widehat{H}_\kappa$ with $\widehat{H}_\kappa$ as defined in Eq. (5); here the prefactor 2 accounts for the fact that by excluding the term corresponding to $\boldsymbol{q}' = \boldsymbol{0}$ in the sum on the RHS of Eq. (86), we have *explicitly* removed the SE of the positively-charged uniform background of charge density en_0 (see text following Eq. (9) above). Throughout this paper we assume

$$g \equiv g_c, \quad \bar{w}(q) \equiv \bar{\mathsf{w}}_{\{\lambda_1,\dots,\lambda_J\}}(q), \tag{89}$$

with $\bar{\mathsf{w}}_{\{\lambda_1,\dots,\lambda_J\}}(q)$ possessing the scaling property

$$\bar{\mathsf{w}}_{\{\alpha\lambda_1,\dots,\alpha\lambda_J\}}(\alpha q) = \alpha^{1-d}\, \bar{\mathsf{w}}_{\{\lambda_1,\dots,\lambda_J\}}(q), \tag{90}$$

that is $\bar{\mathsf{w}}_{\{\lambda_1,\dots,\lambda_J\}}(q)$ is a homogeneous function of q and $\{\lambda_1,\dots,\lambda_J\}$ of degree $1-d$ (for example Ince (1927, p. 10)). Here, as in Eqs. (89) and (90), $\{\lambda_1,\dots,\lambda_J\}$ stands for the set of J parameters on which $\bar{w}(q)$ may depend; these parameters have the same dimension as q, that is inverse length. The property in Eq. (90) is seen to be satisfied by $\bar{w}_c(q)$ in Eq. (88) for which $\bar{\mathsf{w}}_{\{\lambda_1,\dots,\lambda_J\}}(q)$ is equal to $4\pi/(q^2+\kappa^2)$, corresponding to $J=1$ and $\lambda_1 = \kappa$, $\kappa \downarrow 0$; to give another example, for the Yukawa potential in $d=3$, $\bar{\mathsf{w}}_{\{\lambda_1,\dots,\lambda_J\}}(q)$ is equal to $4\pi/(q^2+q_{\text{TF}}^2)$, so that $J=1$ and $\lambda_1 = q_{\text{TF}}$, the Thomas-Fermi screening wavenumber.

In Eq. (86), $\hat{\mathsf{a}}_{\boldsymbol{k};\sigma}$ stands for the annihilation operator corresponding to the particle with spin index σ in the single-particle state $\langle \boldsymbol{r}|\boldsymbol{k}\rangle = \Omega^{-1/2}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})$, characterized by wave-vector $\boldsymbol{k}$; with the creation operator $\hat{\mathsf{a}}^\dagger_{\boldsymbol{k};\sigma}$, which is the Hermitian conjugate of $\hat{\mathsf{a}}_{\boldsymbol{k};\sigma}$, we have the following anticommutation relations (*cf.* Eq. (29) above)

$$\big[\hat{\mathsf{a}}^\dagger_{\boldsymbol{k};\sigma}, \hat{\mathsf{a}}_{\boldsymbol{k}';\sigma'}\big]_+ = \delta_{\sigma,\sigma'}\delta_{\boldsymbol{k},\boldsymbol{k}'},$$
$$\big[\hat{\mathsf{a}}^\dagger_{\boldsymbol{k};\sigma}, \hat{\mathsf{a}}^\dagger_{\boldsymbol{k}';\sigma'}\big]_+ = \big[\hat{\mathsf{a}}_{\boldsymbol{k};\sigma}, \hat{\mathsf{a}}_{\boldsymbol{k}';\sigma'}\big]_+ = 0. \tag{91}$$

With

$$a_0 {:=} \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \equiv \frac{\hbar^2}{m_e g_c} \tag{92}$$

$\mathrm{Im}[\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)]$ to any desired order in $1/\varepsilon$ (see § III.I) alongside the series for $\mathrm{Re}[\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)]$; in practice, however, calculation of the former is *not* as direct as that of the latter (see Eq. (227) below).

[64] The word 'exact' here refers to the exact ϱ_σ, as opposed to $\varrho_{\text{s};\sigma}$, which determines $\Sigma_{\sigma;\infty_0} \equiv \Sigma^{\text{HF}}[\varrho_\sigma]$ (see Eq. (173) below).

the Bohr radius [65] and r_0 the average distance between the particles (independent of their spin indices) in the GS, that is

$$\Omega = \frac{2\pi^{d/2}}{\Gamma(d/2)d}\, r_0^d\, N \iff r_0 = \left(\frac{\Gamma(d/2)d}{2\pi^{d/2} n_0}\right)^{1/d}, \quad (93)$$

where n_0 stands for the total concentration of fermions, defined in Eq. (9), we introduce the *dimensionless* Wigner-Seitz radius

$$r_s := \frac{r_0}{a_0}. \quad (94)$$

In Eq. (93), $\Gamma(x)$ stands for the gamma function (Abramowitz and Stegun 1972, p. 255). [66] Defining the dimension-less volume and wave-vectors according to

$$\bar{\Omega} := \frac{\Omega}{r_0^d}, \quad \bar{\boldsymbol{k}} := r_0 \boldsymbol{k}, \ \text{ etc.}, \quad (95)$$

the Hamiltonian in Eq. (86) can be expressed as follows:

$$\widehat{H} = \frac{\hbar^2}{2m_e a_0^2}\,\frac{2}{r_s^2}\,\widehat{\mathcal{H}}, \quad (96)$$

where

$$\widehat{\mathcal{H}} = \widehat{\mathcal{T}} + \widehat{\mathcal{V}}, \quad (97)$$

in which

$$\widehat{\mathcal{T}} \equiv \sum_{\sigma'} \sum_{\bar{\boldsymbol{k}}'} \frac{1}{2} \bar{k}'^2\, \hat{a}^{\dagger}_{\bar{\boldsymbol{k}}';\sigma'} \hat{a}_{\bar{\boldsymbol{k}}';\sigma'}, \quad (98)$$

and

$$\widehat{\mathcal{V}} \equiv \frac{r_s}{2\bar{\Omega}} \sum_{\sigma_1',\sigma_2'} \sideset{}{'}\sum_{\bar{\boldsymbol{k}}',\bar{\boldsymbol{p}}',\bar{\boldsymbol{q}}'} \bar{w}(\bar{q}') \times \hat{a}^{\dagger}_{\bar{\boldsymbol{k}}'+\bar{\boldsymbol{q}}';\sigma_1'} \hat{a}^{\dagger}_{\bar{\boldsymbol{p}}'-\bar{\boldsymbol{q}}';\sigma_2'} \hat{a}_{\bar{\boldsymbol{p}}';\sigma_2'} \hat{a}_{\bar{\boldsymbol{k}}';\sigma_1'}, \quad (99)$$

where $\bar{w}(\bar{q}')$ stands for $\mathsf{w}_{r_0\lambda_1,\dots,r_0\lambda_J}(r_0\, q')$ (see Eq. (90) above). Above we have introduced

$$\hat{a}_{\bar{\boldsymbol{k}};\sigma} := \hat{\mathsf{a}}_{\bar{\boldsymbol{k}}/r_0;\sigma} \equiv \hat{\mathsf{a}}_{\boldsymbol{k};\sigma}, \quad \hat{a}^{\dagger}_{\bar{\boldsymbol{k}};\sigma} := \hat{\mathsf{a}}^{\dagger}_{\bar{\boldsymbol{k}}/r_0;\sigma} \equiv \hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k};\sigma}. \quad (100)$$

From Eq. (91) it trivially follows that

$$[\hat{a}^{\dagger}_{\bar{\boldsymbol{k}};\sigma}, \hat{a}_{\bar{\boldsymbol{k}}';\sigma'}]_+ = \delta_{\sigma,\sigma'}\delta_{\bar{\boldsymbol{k}},\bar{\boldsymbol{k}}'},$$
$$[\hat{a}^{\dagger}_{\bar{\boldsymbol{k}};\sigma}, \hat{a}^{\dagger}_{\bar{\boldsymbol{k}}';\sigma'}]_+ = [\hat{a}_{\bar{\boldsymbol{k}};\sigma}, \hat{a}_{\bar{\boldsymbol{k}}';\sigma'}]_+ = 0. \quad (101)$$

The Hamiltonian $\widehat{\mathcal{H}}$ is dimensionless and has the interesting property of making explicit that the ratio of the particle-particle interaction energy to the kinetic energy in some eigenstate of the system, is to leading order and up to logarithmic corrections proportional to r_s (whence $r_s \downarrow 0$ corresponds to 'weak' correlation). We mention that [67]

$$\frac{\hbar^2}{2m_e a_0^2} = 1 \text{ Ry} = 13.605\ 6981 \text{ eV} \quad (102)$$

so that, expressing energies in Rydbergs, $\widehat{H}$ is equal to $2/r_s^2$ times $\widehat{\mathcal{H}}$. We define

$$e_0 := \frac{\hbar^2}{m_e a_0^2 r_s^2} \equiv \frac{2}{r_s^2}\,\text{Ry}. \quad (103)$$

In what follows we express energies in units of e_0 and denote the normalized energies by their conventional symbols topped with a single bar, namely $\bar{\varepsilon}_k^{(0)} := \varepsilon_k^{(0)}/e_0$; since in this paper we denote the diagonal elements of the Fourier transform with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$ of functions of $\|\boldsymbol{r} - \boldsymbol{r}'\|$ also through a *single* bar placed on their well-established symbols, below we denote the normalized $\overline{\Sigma}_\sigma(k;\varepsilon)$ by topping this with an additional bar; thus

$$\overline{\overline{\Sigma}}_\sigma(\bar{k};\bar{\varepsilon}) \equiv \frac{\hbar\overline{\Sigma}_\sigma(k;\varepsilon)}{e_0}. \quad (104)$$

Note that it would have been more appropriate to denote the left-hand side (LHS) of Eq. (104) by $\overline{\overline{\hbar\Sigma}}_\sigma(\bar{k};\bar{\varepsilon})$, however we have refrained from doing so for aesthetic reasons. Accordingly, we maintain to use the same convention as in Eq. (104) in the remaining part of this paper.

In view of the expression in Eq. (85), the (dimensionless) single-particle energy $\bar{\varepsilon}_{\bar{k};\sigma}$ is the solution of the following equation (for details see Farid (1999a,c)): [68]

$$\bar{\varepsilon}_{\bar{k}}^{(0)} + \overline{\overline{\Sigma}}_\sigma(\bar{k};\bar{\varepsilon}_{\bar{k};\sigma}) = \bar{\varepsilon}_{\bar{k};\sigma}, \quad (105)$$

where (see Eq. (A35) below)

[65] In dealing with systems in which the fermions are not true elementary particles, but rather long-lived quasi-particles of a host material, the *bare* fermion mass m_e should be replaced by an appropriate effective mass m_e^* and ϵ_0 by $\epsilon_0^* := \epsilon_0\epsilon_{\mathrm{r}}$, with ϵ_{r} the relative dielectric constant of the host material. The effective Bohr radius a_0^* thus obtained, is a more realistic measure (than the Bohr radius a_0) for the lengths relevant to the problem at hand.

[66] Recall that $\Gamma(1/2) = \pi^{1/2}$ and that $\Gamma(1+x) = x\Gamma(x)$.

[67] For m_e we have here used the electron mass in vacuum, equal to $9.109\ 3897\times 10^{-31}$ kg. With a_0 as defined in Eq. (92), our choice for m_e implies that $a_0 = 0.529\ 177\ 249 \times 10^{-10}$ m.

[68] In this equation, the LHS is simply the normalized $\mathcal{E}_{\varsigma;\sigma}(\varepsilon)$, i.e. $\mathcal{E}_{\varsigma;\sigma}(\varepsilon)/e_0$, as introduced in Eq. (84), in which ε is accorded with the (normalized) subscripts of $\mathcal{E}_{\varsigma;\sigma} \equiv \mathcal{E}_{k;\sigma}$, i.e. $\bar{k}$ (see Eq. (95)) and σ.

$$\bar{\varepsilon}^{(0)}_{\bar{k}} := \frac{\varepsilon^{(0)}_k}{e_0} \equiv \frac{1}{2}\,\bar{k}^2. \qquad (106)$$

From the *explicit* linear dependence on r_s of $\widehat{\mathcal{V}}$ in Eq. (99), some general arguments (see footnote 9) and inspection of the explicit results concerning $\{\overline{\overline{\Sigma}}_{\sigma;\infty_m}(\bar{k})\}$, we deduce the following general expressions

$$\overline{\overline{\Sigma}}_{\sigma;\infty_0}(\bar{k}) \equiv r_s\,\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k}), \qquad (107)$$

$$\overline{\overline{\Sigma}}_{\sigma;\infty_1}(\bar{k}) \equiv r_s^2\,\mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k}), \qquad (108)$$

$$\overline{\overline{\Sigma}}_{\sigma;\infty_m}(\bar{k}) \equiv r_s^2\,\mathcal{S}^{(2)}_{\sigma;\infty_m}(\bar{k}) + \dots + r_s^{m+1}\,\mathcal{S}^{(m+1)}_{\sigma;\infty_m}(\bar{k}), \quad m \ge 2, \qquad (109)$$

where $\mathcal{S}^{(p)}_{\sigma;\infty_j}(\bar{k})$, $j = 0, 1, \dots, m$; $p = 1, 2, \dots, m+1$, are *implicit* functions of r_s which do *not* explicitly depend on r_s; the expressions for these functions are readily deduced from the full expression for $\overline{\overline{\Sigma}}_{\sigma;\infty_j}(\bar{k})$. The superscript p in $\mathcal{S}^{(p)}_{\sigma;\infty_j}(\bar{k})$ signifies r_s^p by which it is multiplied. Diagrammatically, $r_s^p \mathcal{S}^{(p)}_{\sigma;\infty_j}(\bar{k})$ is the total contribution to $\overline{\overline{\Sigma}}_{\sigma;\infty_j}(\bar{k})$ due to all pth-order skeleton SE diagrams (for the definition see Luttinger and Ward (1960)) in terms of the *bare* particle-particle interaction function v and the *exact* single-particle GF.

The expression in Eq. (109) does *not* directly apply to $\overline{\overline{\Sigma}}_{\sigma;\infty_m}(\bar{k})$ pertaining to systems of fermions interacting through specifically (but *not* exclusively) $v \equiv v_c$ in $d = 3$. To deal with this case we need to introduce some new notation. Below we do this for general systems, that is including those with possibly inhomogeneous GSs; similar to our considerations in the earlier Sections, below we deal with the coordinate representation of the SE operator.

2. Some notational conventions (general)

Consider the *infinite*-order (asymptotic) series for $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ as presented in Eq. (72), with $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ the coefficient of $1/z^m$. Truncating this series (following the necessary regularizations (see § II.B)) at a finite order, we denote the coefficient of $1/z^m$ by $\widetilde{\Sigma}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'|z)$ and introduce the following decomposition: [69]

$$\widetilde{\Sigma}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'|z) \equiv \Sigma^{\rm r}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}') + \Sigma^{\rm s_b}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}') + \widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z). \qquad (110)$$

Here $\Sigma^{\rm r}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, the 'regular' part of $\widetilde{\Sigma}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'|z)$, consists of *all* contributions to the general expression for $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ that for the interaction function v under consideration, specifically for $v \equiv v_c$, satisfy conditions (A)-(C) in § II.B; $\Sigma^{\rm s_b}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ denotes the totality of functions in $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ that satisfy the requirement (A) in § II.B (that is, they are bounded almost everywhere) but fail to satisfy either (B) or (C), or both (*cf.* Eq. (212) below); finally, $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$ arises from the regularization of the unbounded terms $\Sigma^{\rm s}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$, $p = 2, \dots, m$, in the expression for the original $\Sigma_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$, that is those which fail to satisfy requirement (A) in § II.B (*cf.* Eq. (214) below). In the context of our considerations in this paper, the unbounded terms $\Sigma^{\rm s}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ are those directly associated with the substitution $v \rightharpoonup v_c$ (see later); when not identically vanishing, the actual function $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$ is required to satisfy the following *three* conditions: [70]

$$\frac{1}{\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)} = o(1), \quad \frac{\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)}{z} = o(1), \quad \text{and}$$
$$\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)\ \text{contains \textit{no} decaying parts,} \quad \text{as } |z| \to \infty, \qquad (111)$$

which imply that $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$ may *not* be the full contribution of the pertinent regularized functions (originating from $\Sigma^{\rm s}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$, $p = 2, \dots, m$), but that contribution of these which upon dividing by z^m is asymptotically more dominant than $1/z^{m+1}$ but less dominant than *or* as dominant as (since $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$ *may* consist of a non-vanishing z-independent part; see footnote 31) $1/z^m$ for $|z| \to \infty$. In this paper we denote the *full* contribution arising from the regularization of $\Sigma^{\rm s}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')/z^p$ by $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}';z)$ and that as arising from the regularization of $\Sigma^{\rm s_b}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')/z^p$ (so as to obtain an *integrable* function with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$) by $\widetilde{\Sigma}^{\rm s_b}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}';z)$.

In order to demonstrate the possibility of dependence of $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$ on contributions arising from $\Sigma^{\rm s}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ with $p \le m$ (but specifically with $p < m$), consider the case where, for instance, regularization of a component part of $\Sigma^{\rm s}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ would result in $(-z/\varepsilon_0)^{1/2}\tilde{g}(\boldsymbol{r},\boldsymbol{r}';z)$, in which

$$\tilde{g}(\boldsymbol{r},\boldsymbol{r}';z) \sim \sum_{j=p}^{\infty} \frac{g_{\infty_j}(\boldsymbol{r},\boldsymbol{r}')}{z^j},$$

with $g_{\infty_p}(\boldsymbol{r},\boldsymbol{r}') \not\equiv 0$ and $\{g_{\infty_j}(\boldsymbol{r},\boldsymbol{r}')\| j \ge p\}$ bounded almost everywhere and integrable with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$.

[69] As we shall see, owing to the branch-cut discontinuities of the transcendental functions involved in the pertinent expressions, it is expedient to work with *complex* z and effect the substitution $z \rightharpoonup \varepsilon \pm i\eta$, $\eta \downarrow 0$, only when required in a particular application.

[70] In these expressions are implicit the sufficiency of the Poincaré definition of AS in the context of our work in this paper. See § II.B.

From this we observe that, although $(-z/\varepsilon_0)^{1/2}\tilde{g}(\boldsymbol{r},\boldsymbol{r}';z)$ has direct bearing on $\Sigma^{\rm s}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ (or $\Sigma_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$), it nonetheless contributes to $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$ with $m \geq p$; with reference to the conditions presented in Eq. (111), it is readily observed that this contribution to $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$ is equal to $(-z/\varepsilon_0)^{1/2} g_{\infty_m}(\boldsymbol{r},\boldsymbol{r}')$.

We point out that the requirements in Eq. (111) are necessary insofar as they guarantee that [71]

$$\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z) \sim \Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}') + \frac{\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')}{z} + \frac{\widetilde{\Sigma}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'|z)}{z^2} + \frac{\widetilde{\Sigma}_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}'|z)}{z^3} + \dots \qquad (112)$$

is a *well-ordered* AS for $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ as $|z|\to\infty$, that is the ratio of the $(m+1)$th term to the mth term approaches zero for $|z|\to\infty$ (see § II.B). We should emphasize that the possibility of the first appearance of a z-dependent coefficient function in the *third* leading term on the RHS of Eq. (112) is closely related with $v \equiv v_c$ *and* $d=3$ that we explicitly consider in this paper; to compare, for $v\equiv v_c$ and $d=2$, the first z-dependent coefficient appears in the *second* leading term of the large-$|z|$ AS for $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ (B. Farid, 2001, unpublished).

As discussed in § II.B in detail, $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$ necessarily depends on z, which dependence is *not* polynomial (of finite order), but transcendental. Depending on whether or not the partial infinite summation corresponding to the process of regularization involves contributions with increasing 'powers' of v, $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$ is or is not a transcendental function of the coupling constant of interaction (or of r_s in the systems with uniform and isotropic GSs, discussed above in this Section) respectively; in the latter case, it is a finite-order polynomial of the mentioned coupling constant (here we are solely considering the *explicit* dependence of $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$ on the coupling constant of interaction and not its *implicit* dependence). In any event, even if $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$ should for a given m depend *strictly* polynomially on the interaction coupling constant, the mentioned non-holomorphic dependence of this function upon z gives rise to a transcendental dependence of the single-particle energies on the coupling-constant of interaction.

3. Some intermediate considerations

In the light of the above considerations, we observe that, when $d=3$ and $v\equiv v_c$, $\overline{\overline{\Sigma}}{}^{\rm r}_{\sigma;\infty_m}(\bar{k})$ can be expressed *exactly* as in Eq. (109). Since by definition $\Sigma^{\rm s_b}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ fails to satisfy at least one of the conditions (B) and (C) in § II.B, it follows that the Fourier transform of this function does *not* exist, so that calculation of the AS of the Fourier transform of $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ involving terms of order $1/z^m$ has to be preceded by an infinite summation over a well-specified set of terms pertaining to $\{\Sigma^{\rm s_b}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')/z^p \,\|\, p\geq m\}$, resulting in a function that satisfies conditions (B) and (C) in § II.B (for simplicity, but without loss of generality, here we have assumed that $\Sigma^{\rm s_b}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ has not already been accounted for in the process of regularization of $\Sigma^{\rm s_b}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$, with $p<m$; see later); we denote this function, which in addition to $\boldsymbol{r}$ and $\boldsymbol{r}'$ also depends on z, by $\widetilde{\Sigma}^{\rm s_b}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}';z)$. Only *after* the Fourier transformation of this function, can the contribution to the desired large-$|z|$ AS of the Fourier transform of $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$, as originating from $\Sigma^{\rm s_b}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, be calculated. Precisely as is the case with the determination of $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$, where account has to be taken of the asymptotic contributions due to functions arising from the regularization of unbounded contributions to $\Sigma_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ with $p<m$ (see text succeeding Eq. (112) above), here also the coefficient of $1/z^m$ in a finite-order AS for the Fourier transform of $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$, $|z|\to\infty$, can in principle involve contributions from the large-$|z|$ AS of the Fourier transform of $\widetilde{\Sigma}^{\rm s_b}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}';z)$ with $p<m$. Since in our considerations (specialized to $v\equiv v_c$ in $d=3$) $\Sigma_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ are fully regular (in the sense of § II.B) for $p=0,1$, it follows that in determining the coefficient of $1/z^2$ in the large-$|z|$ AS for the Fourier transform of $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$, there are *no* contributions to be taken into account that would otherwise originate from the large-$|z|$ AS of the Fourier transform of $\widetilde{\Sigma}^{\rm s_b}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}';z)$ with $p<2$. In Appendix H we determine both $\widetilde{\Sigma}^{\rm s_b}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}';z)$ and the expressions for the relevant terms in the large-$|z|$ AS of the double Fourier transform of this function with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$. For uniform systems of spin-1/2 fermions, we deduce the *exact* leading-order term pertaining to the fully-interacting system, while for the same system we calculate the second term within the framework of the 'single Slater-determinant' approximation (SSDA) (see Appendix C).

Our considerations in Appendices F, G and H lead to the following results: [72]

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[71] Within the context of our considerations in this paper, $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')$ and $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ are strictly regular, so that the expression in Eq. (111) has relevance to $m\geq 2$, $m=2$ being specifically significant for v_c in $d=3$.

[72] In order to prevent confusion, below we replace the $\bar{k}$ argument of functions that do *not* depend on $\bar{k}$ (i.e. those that are naturally associated with *local* operators) by "·". We point out that since $\Sigma^{\rm s_b}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ is *non*-integrable (although it is bounded almost everywhere), for the 'coefficient' of $1/z^m$ in the *regularized* large-$|z|$ AS of the double Fourier transform of $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ with respect to $\boldsymbol{r}$ and

$$\overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\bar{k}\|\bar{z}) = r_s^3\big\{ -\frac{3}{2}\ln(-\bar{z}/r_s) + \mathcal{S}^{\mathrm{s_b}(3)}_{\sigma;\infty_2}(\bar{k})\big\}, \quad (113)$$

$$\overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s}}_{\sigma;\infty_2}(\cdot\|\bar{z}) = \frac{3\,r_s^2}{\sqrt{2}}\,\big[n_{0;\bar{\sigma}}/n_0 - n_{0;\sigma}/n_0\big]\,(-\bar{z})^{1/2} + r_s^3\big\{3\ln(-\bar{z}/r_s^2) + \mathcal{S}^{\mathrm{s}(3)}_{\sigma;\infty_2}\big\}, \quad (114)$$

where [73]

$$\mathcal{S}^{\mathrm{s_b}(3)}_{\sigma;\infty_2}(\bar{k}) = \frac{3}{2}(\gamma-1) + 3\int \frac{\mathrm{d}^3k'}{(2\pi)^3}\,\frac{\overline{\varrho}{}^{\mathrm{h}}_{\sigma}(\|\boldsymbol{k}'\|)}{n_0}\,\ln\big(\|\bar{\boldsymbol{k}} - r_0\boldsymbol{k}'\|\big)\,; \quad (115)$$

$$\mathcal{S}^{\mathrm{s}(3)}_{\sigma;\infty_2} = 3\ln(R/a_0) + 3\int_0^\infty \mathrm{d}r\,\big[\frac{\Theta(r-R)}{r} + \frac{1}{g_c n_0}\,\Lambda^{\mathrm{h}}(r)\big], \quad (116)$$

in which a_0 is the Bohr radius defined in Eq. (92) and (see Eq. (F143))

$$R \gg \frac{e^2}{4\pi\epsilon_0\,|z|}. \quad (117)$$

For $\overline{\varrho}{}^{\mathrm{h}}_{\sigma}$, Λ^{h} and R see in particular Eqs. (J3), (F134) and (F142) respectively; for the significance of superscript h see Eq. (F9). Note that $\overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s}}_{\sigma;\infty_2}(\cdot\|\bar{z})$ in Eq. (114) indeed satisfies the requirements in Eq. (111) and that the first contribution on the RHS of Eq. (114) is identically vanishing for $n_\sigma \equiv n_{\bar{\sigma}}$ (see Appendix G). Combining the results in Eqs. (113) and (114), we have

$$\begin{aligned}\overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s_b}\oplus\mathrm{s}}_{\sigma;\infty_2}(\bar{k}\|\bar{z}) &:= \overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\bar{k}\|\bar{z}) + \overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s}}_{\sigma;\infty_2}(\cdot\|\bar{z})\\ &= \frac{3\,r_s^2}{\sqrt{2}}\,\big[n_{0;\bar{\sigma}}/n_0 - n_{0;\sigma}/n_0\big]\,(-\bar{z})^{1/2}\\ &\quad + r_s^3\big\{\frac{3}{2}\,\ln(-\bar{z}/r_s^3) + \mathcal{S}^{\mathrm{s_b}\oplus\mathrm{s}(3)}_{\sigma;\infty_2}(\bar{k})\big\}, \quad (118)\end{aligned}$$

where

$$\mathcal{S}^{\mathrm{s_b}\oplus\mathrm{s}(3)}_{\sigma;\infty_2}(\bar{k}) := \mathcal{S}^{\mathrm{s_b}(3)}_{\sigma;\infty_2}(\bar{k}) + \mathcal{S}^{\mathrm{s}(3)}_{\sigma;\infty_2}. \quad (119)$$

For completeness, we present the following expression (see Appendix H), to be compared with that in Eq. (115):

$$\begin{aligned}\mathcal{S}^{\mathrm{s_b}(3)}_{\sigma;\infty_2}(\bar{k})\Big|_{\mathrm{s}} &= \frac{3}{2}(\gamma-1) + \frac{3}{16}\big[(\bar{k}/\bar{k}_F)^2 - 17/3\big]\\ &-\frac{3}{32}\frac{\bar{k}_F}{\bar{k}}\,\Big[\big(1-\bar{k}/\bar{k}_F\big)^3\big(3+\bar{k}/\bar{k}_F\big)\,\ln(|\bar{k}_F - \bar{k}|)\\ &\quad -\big(1+\bar{k}/\bar{k}_F\big)^3\big(3-\bar{k}/\bar{k}_F\big)\,\ln(|\bar{k}_F + \bar{k}|)\Big]. \quad (120)\end{aligned}$$

In what follows we mainly deal with the solution of the equation for single-particle energies, i.e. Eq. (105). Below we shall for the large part deal with the general case where the complications such as those associated with $v \equiv v_c$ in $d=3$ are not present; at places, however, we shall make comments relevant to v_c in $d=3$. We shall consider two regimes, corresponding to $r_s \lesssim 1$, and $r_s > 1$, the weak- and intermediate-coupling regime and strong-coupling regime respectively.

4. The weak- and intermediate-coupling regimes

Here we consider the solution of Eq. (105) in the weak- and intermediate-coupling regimes, corresponding to $r_s < 1$ and $r_s \approx 1$ respectively. To this end, we first deal with $\overline{\overline{\Sigma}}_\sigma(\bar{k};\bar{\varepsilon})$, corresponding to an *unspecified* $\bar{\varepsilon}$, for which following Eqs. (72), (107), (108) and (109), we have

$$\overline{\overline{\Sigma}}_\sigma(\bar{k};\bar{\varepsilon}) = r_s\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k}) + \sum_{j=2}^{\infty} r_s^j \sum_{p=j-1}^{\infty} \frac{\mathcal{S}^{(j)}_{\sigma;\infty_p}(\bar{k})}{\bar{\varepsilon}^p}. \quad (121)$$

We note that

$$r_s^j \sum_{p=j-1}^{\infty} \frac{\mathcal{S}^{(j)}_{\sigma;\infty_p}(\bar{k})}{\bar{\varepsilon}^p} \equiv \overline{\overline{\Sigma}}{}^{(j)}_\sigma(\bar{k};\bar{\varepsilon}), \quad (122)$$

where $\overline{\overline{\Sigma}}{}^{(j)}_\sigma(\bar{k};\bar{\varepsilon})$ stands for the total contribution of the jth-order SE terms of the *exact* $\overline{\overline{\Sigma}}_\sigma(\bar{k};\bar{\varepsilon})$ within the framework of many-body perturbation theory in terms of the *bare* particle-particle interaction function v and the *exact* single-particle GF (see § I.B and the text following Eq. (109) above); diagrammatically, $\overline{\overline{\Sigma}}{}^{(j)}_\sigma(\bar{k};\bar{\varepsilon})$ is described by the complete set of jth-order skeleton SE diagrams. Equation (121) makes explicit that in order for a perturbative approximation correctly to reproduce $\Sigma_{\sigma;\infty_m}$, it is necessary to employ the *full* perturbation series to order $m+1$ (inclusive) (see § I.B), following the observation that the lower boundary of the sum on the LHS of Eq. (122) is $j-1$. This rule is of course meaningful only when the pertinent finite-order perturbation series

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$\boldsymbol{r}'$, that is $\overline{\overline{\widetilde{\Sigma}}}_\sigma(\boldsymbol{q},\boldsymbol{q}';z)$, which we denote by $\overline{\overline{\widetilde{\Sigma}}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}'|z)$ (*cf.* Eq. (112)), we have (*cf.* Eq. (110)) $\overline{\overline{\widetilde{\Sigma}}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}'|z) = \overline{\overline{\Sigma}}{}^{\mathrm{r}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}') + \overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}'\|z) + \overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}'\|z)$. Here both $\overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}'\|z)$ and $\overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}'\|z)$ are required to satisfy the three generic conditions specified in Eq. (111). The origin of the dependence on z of $\overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}'\|z)$ should be evident (see § II.B). When appropriate, we denote the z-independent contribution to $\overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}'\|z)$ by $\overline{\overline{\Sigma}}{}^{\mathrm{s_b}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}')$ (see text following Eq. (H11)). Thus, $r_s^3\,\mathcal{S}^{\mathrm{s_b}(3)}_{\sigma;\infty_2}(\bar{k})$ in Eq. (113) represents what we could have denoted as $\overline{\overline{\Sigma}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\bar{k})$. We adopt a similar convention concerning $\overline{\overline{\widetilde{\Sigma}}}{}^{\mathrm{s}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}'\|z)$ (*cf.* Eq. (114)).

[73] Here γ stands for the Euler number (see Eq. (F153)).

do *not* involve unbounded contributions, thus excluding the cases corresponding to $v \equiv v_c$ in $d = 3$ (except when only the first-order series is to be dealt with) for which this statement can be appropriately generalized.

The expression in Eq. (121) is of considerable importance, for it makes explicit that for $|\bar{\varepsilon}| \gg 1$ we can write

$$\sum_{p=j-1}^{\infty} \frac{\mathcal{S}^{(j)}_{\sigma;\infty_p}(\bar{k})}{\bar{\varepsilon}^p} \sim \frac{\mathcal{S}^{(j)}_{\sigma;\infty_{j-1}}(\bar{k})}{\bar{\varepsilon}^{j-1}} + \frac{\mathcal{S}^{(j)}_{\sigma;\infty_j}(\bar{k})}{\bar{\varepsilon}^j} + \dots, \quad (123)$$

and consequently

$$\sum_{j=2}^{\infty} r_s^j \sum_{p=j-1}^{\infty} \frac{\mathcal{S}^{(j)}_{\sigma;\infty_p}(\bar{k})}{\bar{\varepsilon}^p} \sim r_s \sum_{j=2}^{\infty} \frac{\mathcal{S}^{(j)}_{\sigma;\infty_{j-1}}(\bar{k})}{(\bar{\varepsilon}/r_s)^{j-1}} + \sum_{j=2}^{\infty} \frac{\mathcal{S}^{(j)}_{\sigma;\infty_j}(\bar{k})}{(\bar{\varepsilon}/r_s)^j} + \dots. \quad (124)$$

The RHS of this expression shows that a further simplification can be achieved when $|\bar{\varepsilon}| \gg r_s$, under which condition one can write

$$r_s \sum_{j=2}^{\infty} \frac{\mathcal{S}^{(j)}_{\sigma;\infty_{j-1}}(\bar{k})}{(\bar{\varepsilon}/r_s)^{j-1}} \sim r_s \frac{\mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k})}{\bar{\varepsilon}/r_s} + r_s \frac{\mathcal{S}^{(3)}_{\sigma;\infty_2}(\bar{k})}{(\bar{\varepsilon}/r_s)^2} + \dots, \quad (125)$$

$$\sum_{j=2}^{\infty} \frac{\mathcal{S}^{(j)}_{\sigma;\infty_j}(\bar{k})}{(\bar{\varepsilon}/r_s)^j} \sim \frac{\mathcal{S}^{(2)}_{\sigma;\infty_2}(\bar{k})}{(\bar{\varepsilon}/r_s)^2} + \dots. \quad (126)$$

With $\bar{\varepsilon} {:=} \varepsilon/e_0$, since (see Eq. (103))

$$\bar{\varepsilon} = \frac{\varepsilon}{2\,\mathrm{Ry}}\, r_s^2 \iff \frac{\bar{\varepsilon}}{r_s} = \frac{\varepsilon}{2\,\mathrm{Ry}}\, r_s, \quad (127)$$

we observe that there are a number different possibilities for satisfying both $|\bar{\varepsilon}| \gg 1$ and $|\bar{\varepsilon}|/r_s \gg 1$. In the range of metallic densities, where $2 \lesssim r_s \lesssim 6$ (specifically, where $r_s > 1$, corresponding to the 'intermediate-coupling' *regime*), we observe that it is the condition $|\bar{\varepsilon}|/r_s \gg 1$ that determines the minimum $|\bar{\varepsilon}|$ beyond which both $|\bar{\varepsilon}| \gg 1$ and $|\bar{\varepsilon}|/r_s \gg 1$ are satisfied. For Na with $r_s \approx 4$, $|\varepsilon|$ should exceed $\frac{1}{2}$ Ry in order for $|\bar{\varepsilon}|/r_s > 1$; for $|\varepsilon| \gtrsim \frac{1}{2}$ Ry, however, we have $|\bar{\varepsilon}| \gtrsim 4$. In the weak-coupling *regime* where $r_s < 1$, on the other hand, it is the condition $|\bar{\varepsilon}| \gg 1$ that determines the minimum $|\bar{\varepsilon}|$ required for the satisfaction of both $|\bar{\varepsilon}| \gg 1$ and $|\bar{\varepsilon}|/r_s \gg 1$.

Assuming $|\bar{\varepsilon}| \gg \max(1, r_s)$, we can combine the results in Eqs. (121), (124), (125) and (126) and obtain

$$\overline{\overline{\Sigma}}_{\sigma}(\bar{k};\bar{\varepsilon}) \sim r_s \mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k}) + r_s^2\, \frac{\mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k})}{\bar{\varepsilon}} + r_s^2\, \frac{\mathcal{S}^{(2)}_{\sigma;\infty_2}(\bar{k})}{\bar{\varepsilon}^2} + r_s^3\, \frac{\mathcal{S}^{(3)}_{\sigma;\infty_2}(\bar{k})}{\bar{\varepsilon}^2} + \dots. \quad (128)$$

With reference to the considerations leading to the result in Eq. (128), one readily obtains the counterpart of the expression in Eq. (128) for the case corresponding to $v \equiv v_c$ in $d = 3$: since singular contributions to $\overline{\overline{\Sigma}}_{\sigma;\infty_m}(\bar{k}|z)$, as arising from $\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s}}_{\sigma;\infty_m}(\bar{k}\|\bar{z})$, exist only for $m \geq 2$ (here we are employing the notational convention introduced in § III.E.2, for the diagonal components of the SE operator in the momentum representation; by symmetry, the off-diagonal components are identically vanishing), the first two terms on the RHS of Eq. (128) remain unchanged (*qua* form) in the case corresponding to $v \equiv v_c$ and $d = 3$ (*cf.* Eq. (112)). Denoting the counterparts of $\mathcal{S}^{(2)}_{\sigma;\infty_2}(\bar{k})$ and $\mathcal{S}^{(3)}_{\sigma;\infty_2}(\bar{k})$, as arising from $\overline{\overline{\Sigma}}{}^{\mathrm{r}}_{\sigma;\infty_2}(\bar{k})$ (the normalized diagonal component of the momentum representation of $\Sigma^{\mathrm{r}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ introduced in Eq. (110)), by $\mathcal{S}^{\mathrm{r}(2)}_{\sigma;\infty_2}(\bar{k})$ and $\mathcal{S}^{\mathrm{r}(3)}_{\sigma;\infty_2}(\bar{k})$ respectively, from Eqs. (110), (112) and (118) for $|\bar{z}| \gg \max(1, r_s)$ we obtain (*cf.* Eq. (128))

$$\widetilde{\overline{\overline{\Sigma}}}_{\sigma}(\bar{k};\bar{z}) \sim r_s \mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k}) + r_s^2\, \frac{\mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k})}{\bar{z}} + r_s^2\, \frac{\mathcal{S}^{\mathrm{r}(2)}_{\sigma;\infty_2}(\bar{k}) + 3\big[n_{0;\bar{\sigma}}/n_0 - n_{0;\sigma}/n_0\big]\,(-\bar{z}/2)^{1/2}}{\bar{z}^2} + r_s^3\, \frac{\mathcal{S}^{\mathrm{r}(3)}_{\sigma;\infty_2}(\bar{k}) + \mathcal{S}^{\mathrm{s_b}\oplus\mathrm{s}}_{\sigma;\infty_2}(\bar{k}) + (3/2)\,\ln(-\bar{z}/r_s^3)}{\bar{z}^2} + \dots. \quad (129)$$

The results in Eqs. (128) and (129) are evidently the appropriate expressions for the determination of the single-particle excitation energies $\{\bar{\varepsilon}_{\bar{k};\sigma}\}$ in the 'weak-coupling' *regime*, that is $r_s < 1$ (note the increasing powers of r_s), at sufficiently large values of $|\bar{\varepsilon}| = |\bar{\varepsilon}_{\bar{k};\sigma}|$. On the other hand, since in arriving at the results in Eqs. (128) and (129), the basic assumption has been $|\bar{\varepsilon}| \gg \max(1, r_s)$, these are equally applicable in the intermediate-coupling regime (let us say, for r_s in the range corresponding to metallic densities), and even strong-coupling regime, in exchange for larger values of $|\bar{\varepsilon}| = |\bar{\varepsilon}_{\bar{k};\sigma}|$, as implied by $|\bar{\varepsilon}| \gg \max(1, r_s)$.

In the weak-coupling *limit* corresponding to $r_s \ll 1$, the terms on the RHSs of Eqs. (128) and (129) which are proportional to r_s^3 can be neglected in comparison with those proportional to r_s^2. In turn, the latter contributions are negligible in comparison with $r_s \mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k})$. The proportionality with r_s of this term implies that Eq. (105) in conjunction with Eqs. (128) and (129) correctly yields $\bar{\varepsilon}_{\bar{k};\sigma} \to \bar{\varepsilon}^{(0)}_{\bar{k}}$ as $r_s \downarrow 0$. It is important to note that neglect of the contributions proportional to r_s^3 on the RHSs of Eqs. (128) and (129), results in a notable simplification in the calculations, a fact that can be readily verified through inspecting the explicit expressions for $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ and $\Sigma^{\mathrm{r}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ in Eqs. (199) and (211) respectively, and eliminating all terms herein that involve the third power of the coupling constant of v.

Calculation of $\bar{\varepsilon}_{\bar{k};\sigma}$ from Eq. (105) in which $\overline{\overline{\Sigma}}_\sigma(\bar{k};\bar{\varepsilon}_{\bar{k};\sigma})$ is replaced by a *finite-order* series, such as that in Eq. (128) or in Eq. (129), involves the interesting aspect that unlike $\bar{\varepsilon}$, $\bar{\varepsilon}_{\bar{k};\sigma}$ is *not* a free parameter so that in principle, in particular when r_s is *not* truly small, one does not have an *a priori* reason for considering the solution as necessarily accurate. This can, however, be established through *a posteriori* verifying whether the calculated $\bar{\varepsilon}_{\bar{k};\sigma}$, for a given $\bar{k}$, satisfies the underlying assumption $|\bar{\varepsilon}_{\bar{k};\sigma}| \gg \max(1, r_s)$. Since, however, $\bar{\varepsilon}_{\bar{k};\sigma} \sim \bar{\varepsilon}_{\bar{k}}^{(0)}$ for $\bar{k} \gg \bar{k}_F$, the sufficiency of Eqs. (128) and (129) for $\bar{k} \gg \bar{k}_F$ is guaranteed by $\bar{\varepsilon}_{\bar{k}}^{(0)} \gg 1$.

Our above considerations concerning the accuracy of finite-order AS for $\overline{\overline{\Sigma}}_\sigma(\bar{k};\bar{\varepsilon})$ rely solely on the *explicit* dependences on r_s of various terms, disregarding the possibility that these terms, when stripped off of these dependences, can themselves be small or large or that they may exhibit considerable variation with respect to $\bar{k}$, so that accuracy of the above expressions may also depend on the value of $\bar{k}$ considered. In this connection it is instructive to consider $\overline{\overline{\Sigma}}_{\sigma;\infty_0}(\bar{k})$ within the framework of the SSDA of the GS wavefunction; for simplicity, we deal with a system of spin-1/2 fermions in the paramagnetic phase. For this we have (below the subscript 's' is indicative of this approximation) [74] [75]

$$\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k})\Big|_{\mathrm{s}} = -\frac{2}{\pi}\left(\frac{9\pi}{4}\right)^{1/3} \mathsf{F}(\bar{k}/\bar{k}_F), \quad \sigma = \pm 1/2, \quad (130)$$

where

$$\mathsf{F}(x) := \frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right| \sim \frac{1}{3x^2} + \frac{1}{15x^4} + \dots, \quad |x| \to \infty. \quad (131)$$

With $\mathsf{F}(0) = 1$ and $\mathsf{F}(1) = 1/2$, one observes a significant dependence on $\bar{k}$ of $\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k})|_{\mathrm{s}}$ for $\bar{k} \in [0, \bar{k}_F]$. In Appendix F we calculate the contribution of the *local* part of $\Sigma_{\sigma;\infty_1}$ to $\mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k})$ within the framework of the SSDA, which amounts to $(2\mathsf{a}_{\mathrm{s}}/\pi)\,(9\pi/4)^{2/3} \approx 1.32$ (see Eq. (F67)); the sign of this quantity is opposite to that of $\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k})|_{\mathrm{s}}$ in Eq. (130) and its value is almost equal to the absolute value of $\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k})|_{\mathrm{s}}$ for small values of $\bar{k}$.

With reference to the series in Eq. (121), whether this be considered as an AS of $\overline{\overline{\Sigma}}_\sigma(\bar{k};\bar{\varepsilon})$ for $|\bar{\varepsilon}| \to \infty$ or one for $r_s \to 0$, we observe that for $\bar{\varepsilon} > 0$ we *may* have to do with an *alternating* AS. [76] If this turns out to be the case, then the *theory of terminants* (Dingle 1973, chapter XXI) (see also Copson 1965 for an exposition of the method of Stieltjes, according to which the last incorporated term in an alternating asymptotic series is simply multiplied by 1/2) can be fruitfully employed for deducing very accurate results for $\overline{\overline{\Sigma}}_\sigma(\bar{k};\bar{\varepsilon})$ through appropriately terminating the AS.

5. *The strong-coupling regime*

Making use of Eqs. (107) - (109), we can rewrite Eq. (105) as follows: [77]

$$\bar{\varepsilon}_{\bar{k}}^{(0)} + r_s F_{1;\sigma;r_s}(\bar{\varepsilon}_{\bar{k};\sigma}/r_s;\bar{k}) + \sum_{j=2}^{\infty} \frac{1}{r_s^{j-2}} F_{j;\sigma;r_s}(\bar{\varepsilon}_{\bar{k};\sigma}/r_s;\bar{k}) = \bar{\varepsilon}_{\bar{k};\sigma}, \quad (132)$$

where

$$F_{1;\sigma;r_s}(x;\bar{k}) := \sum_{p=0}^{\infty} \frac{\mathcal{S}^{(p+1)}_{\sigma;\infty_p}(\bar{k})}{x^p}, \quad (133)$$

$$F_{j;\sigma;r_s}(x;\bar{k}) := \sum_{p=j}^{\infty} \frac{\mathcal{S}^{(p+2-j)}_{\sigma;\infty_p}(\bar{k})}{x^p}, \quad j \geq 2. \quad (134)$$

The subscript r_s in $F_{j;\sigma;r_s}(x;\bar{k})$, $j = 1, 2, \dots$, signifies the *implicit* dependence on r_s of $F_{j;\sigma;r_s}(x;\bar{k})$. As long as the sums in Eqs. (132) - (134) are *not* truncated (or at most only partially truncated so that complete sets of unbounded contributions are accounted for), the result in Eq. (132) is also applicable to the case corresponding to $v \equiv v_c$ in $d = 3$. Note that Eq. (132) is exact, so that it equally applies to small values of r_s; it is not difficult to verify that for $r_s \to 0$, the expression in Eq. (121) is directly deduced from Eq. (132) (and *vice versa*); consider,

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[74] $(2/\pi)(9\pi/4)^{1/3} \approx 1.22$.

[75] Restricting the AS on the RHSs of Eqs. (128) and (129) to their leading term $r_s\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k})$, while replacing $\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k})$ by the expression on the RHS of Eq. (130) below, one obtains $\overline{\overline{\Sigma}}{}^{\mathrm{HF}}_{\mathrm{s}}(\bar{k})$, the Hartree-Fock SE (within the framework of the SSDA). The single-particle excitation energy corresponding to this, following Eqs. (105) and (106), is equal to $\bar{k}^2/2 - (2/\pi)\bar{k}_F\, r_s\, \mathsf{F}(\bar{k}/\bar{k}_F)$ which is exactly the single-particle energy dispersion according to the conventional Hartree-Fock scheme (for example Ashcroft and Mermin (1981, p. 334)). Here, $\bar{k}_F = (9\pi/4)^{1/3}$.

[76] For $\bar{\varepsilon} \to -\infty$, one should consider the AS at issue as consisting of two sub-series, one involving the *even* powers of $\bar{\varepsilon}$ and one involving the *odd* powers of $\bar{\varepsilon}$, each of which *may* be alternating.

[77] Evidently, $\overline{\overline{\Sigma}}_\sigma(\bar{k};\bar{\varepsilon}) = r_s F_{1;\sigma;r_s}(\bar{\varepsilon}/r_s;\bar{k}) + \sum_{j=2}^{\infty} r_s^{-j+2} F_{j;\sigma;r_s}(\bar{\varepsilon}/r_s;\bar{k})$ for arbitrary $\bar{\varepsilon}$ (*cf.* Eq. (121)). This expression is seen to be ideally suited to use when $\bar{\varepsilon}$ takes on a finite value and $r_s \to \infty$. Proceeding along the lines of § III.B, one can easily deduce a similar expression which is appropriate for the region $\bar{\varepsilon} \to \bar{\varepsilon}_F$.

for instance, the terms in Eq. (121) up to and including the *explicit* quadratic order in r_s; making use of the asymptotic results for $|x| \to \infty$ (corresponding to $r_s \to 0$)

$$F_{1;\sigma;r_s}(x;\bar{k}) \sim \mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k}) + \frac{1}{x}\,\mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k}), \tag{135}$$

$$F_{j;\sigma;r_s}(x;\bar{k}) \sim \frac{1}{x^j}\,\mathcal{S}^{(2)}_{\sigma;\infty_j}(\bar{k}), \quad j \ge 2, \tag{136}$$

which are directly deduced from the expressions in Eqs. (133) and (134), Eq. (132) is readily shown to transform into Eq. (121) to the appropriate order.

From Eq. (132) we observe that for $\bar{\varepsilon}_{\bar{k};\sigma}$ to be bounded as $r_s \to \infty$ (the 'strong-coupling' *limit*), it is necessary that the following conditions be met:

$$\lim_{r_s\to\infty} r_s F_{1;\sigma;r_s}(\bar{\varepsilon}_{\bar{k};\sigma}/r_s;\bar{k}) = \phi_{1;\sigma}(\bar{k}), \tag{137}$$

$$\lim_{r_s\to\infty} r_s^{j-2} F_{j;\sigma;r_s}(\bar{\varepsilon}_{\bar{k};\sigma}/r_s;\bar{k}) = \phi_{j;\sigma}(\bar{k}), \quad j \ge 2, \tag{138}$$

where $\{\phi_{j;\sigma}(\bar{k})\}$ stands for a set of bounded functions of $\bar{k}$; the dependence of these functions on $\bar{k}$ may be partly due to that of $\bar{\varepsilon}_{\bar{k};\sigma}$ on $\bar{k}$. As can be readily inferred from the relationship between $\mathcal{S}^{(p)}_{\sigma;\infty_m}$ and the contributions of the skeleton SE diagrams (see text following Eq. (122) above), $\{F_{j;\sigma;r_s}(x;\bar{k})\}$ are *all* bounded functions of r_s for *all* r_s. Therefore, the most stringent condition as implied by the requirement that $\bar{\varepsilon}_{\bar{k};\sigma}$ be finite in the strong-coupling *limit*, is that given in Eq. (137), with $\phi_{1;\sigma}(\bar{k})$ *bounded*, implying that $F_{1;\sigma;r_s}(\bar{\varepsilon}_{\bar{k};\sigma}/r_s;\bar{k})$ should decay at the slowest like $1/r_s$ as $r_s \to \infty$; with $F_{1;\sigma;r_s}(\bar{\varepsilon}_{\bar{k};\sigma}/r_s;\bar{k})$ decaying in this limit like $1/r_s^{\eta}$ with $\eta > 1$, we have $\phi_{1;\sigma}(\bar{k}) \equiv 0$. Thus, to the leading order in $1/r_s$ we have

$$\bar{\varepsilon}_{\bar{k};\sigma} \sim \bar{\varepsilon}^{(0)}_{\bar{k}} + \phi_{1;\sigma}(\bar{k}) + \phi_{2;\sigma}(\bar{k}), \quad r_s \to \infty, \tag{139}$$

where $\phi_{1;\sigma}(\bar{k})$ *may* be identically vanishing. We note that from knowledge that, for sufficiently large value of r_s, the GS of the system under consideration is *not* uniform but a Wigner crystal, it follows that the result in Eq. (139) will be valid for r_s less than a critical value, $r_s^{\rm c}$, which for spin-1/2 fermions in $d = 3$ is of the order of 10^2 (Ceperley and Alder 1980, Herman and March 1984, Ortiz, *et al.* 1999). We point out that by the Seitz (1940, pp. 343 and 344) theorem, [78] the value of $\bar{\varepsilon}_{\bar{k};\sigma} - \bar{\varepsilon}^{(0)}_{\bar{k}}$ is fixed at $\bar{k} = \bar{k}_{F;\sigma}$, so that in the limit $r_s \to \infty$ (to be precise, $r_s \to r_s^{\rm c}$), knowledge of $\phi_{1;\sigma}(\bar{k}_F)$ is sufficient to determine $\phi_{2;\sigma}(\bar{k}_F)$, and vice versa.

The above results clearly demonstrate the complexity of calculation of $\bar{\varepsilon}_{\bar{k};\sigma}$ in the 'strong-coupling' regime in comparison with that in the 'weak-coupling' one. It is however possible that some scheme that interpolates the weak-coupling results with those of the strong-coupling *limit*, may turn out to be accurate for use at all r_s. Consider *for instance* the following *interpolation* expressions:

$$F^{\rm int.}_{1;\sigma;r_s}(x;\bar{k}) = \frac{x\,\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k})}{x+1} + \frac{x\,[\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k}) + \mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k})]}{x^2+1}, \tag{140}$$

$$F^{\rm int.}_{j;\sigma;r_s}(x;\bar{k}) = \frac{\mathcal{S}^{(2)}_{\sigma;\infty_j}(\bar{k})}{x^j + \gamma_\sigma(r_s)}, \quad j \ge 2, \tag{141}$$

where the constant $\gamma_\sigma(r_s)$ is to be chosen such that $\bar{\varepsilon}_F - \bar{\varepsilon}^{(0)}_F = \mu_{\rm xc}(r_s)$, or $\phi_{1;\sigma}(\bar{k}_F) + \phi_{2;\sigma}(\bar{k}_F) = \mu_{\rm xc}(r_s \to \infty)$, be satisfied (see footnote 78). Note that for $|x| \to \infty$, the expressions in Eqs. (140) and (141) satisfy those in Eqs. (135) and (136) respectively and that, according to these interpolation formulae,

$$\phi_{1;\sigma}(\bar{k}) = \big\{2\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k}) + \mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k})\big\}\,\bar{\varepsilon}_{\bar{k};\sigma}, \tag{142}$$

$$\phi_{2;\sigma}(\bar{k}) = \frac{1}{\gamma_\sigma(\infty)}\,\mathcal{S}^{(2)}_{\sigma;\infty_2}(\bar{k}), \tag{143}$$

which in combination with Eq. (139) yield

$$\bar{\varepsilon}_{\bar{k};\sigma} \sim \frac{\bar{\varepsilon}^{(0)}_{\bar{k}} + \mathcal{S}^{(2)}_{\sigma;\infty_2}(\bar{k})/\gamma_\sigma(\infty)}{1 - [2\mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k}) + \mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k})]}, \quad r_s \to \infty. \tag{144}$$

With reference to our considerations following Eq. (131) above, one observes that, for small values of $\bar{k}$ and within the framework of the SSDA, the denominator of the expression on the RHS of Eq. (144) is approximately equal to two.

Above we have dealt with uniform and isotropic systems of fermions, interacting through a bounded and short-range two-body potential v. As we have indicated at the outset of this Section, for $v \equiv v_c$ in $d = 3$, Eq. (132) retains its validity provided *all* the summations, including those in Eqs. (133) and (134), are fully or partially

[78] With $E_0(n_0)$ denoting the GS total energy per particle of a uniform system and n_0 the total particle concentration (see Eq. (9)), the Seitz theorem (Seitz 1940, pp. 343 and 344) reads $\varepsilon_F = {\rm d}[n_0 E_0(n_0)]/{\rm d}n_0$. Assuming the system to be in the paramagnetic state ($\bar{k}_{F;\sigma} = \bar{k}_{F;\bar{\sigma}}$), with $E_0(n_0) \equiv E_{\rm kin}(n_0) + E_{\rm xc}(n_0)$, where $E_{\rm kin}(n_0) = \frac{3}{5}\varepsilon_F^{(0)}$ and $E_{\rm xc}(n_0)$ the exchange-correlation energy per particle, we have $\varepsilon_F - \varepsilon_F^{(0)} {=:} \mu_{\rm xc}(r_s) \equiv {\rm d}[n_0 E_{\rm xc}(n_0)]/{\rm d}n_0$ (*cf.* Eq. (A54)). We note in passing that $\varepsilon_F = \varepsilon_F^{(0)} + \mu_{\rm xc}(r_s)$ amounts to the well-known statement that the energy of the highest-occupied single-particle wavefunction of the Kohn-Sham (1965) equation, which features within the framework of the density-functional theory (Hohenberg and Kohn 1964) (for example Dreizler and Gross (1990)), coincides with the Fermi energy of the interacting system.

(but to some *infinite* order; see above) taken into account. However, Eq. (109) is no longer valid, in consequence of containing un-compensated unbounded contributions associated with $\overline{\overline{\Sigma}}_{\sigma;\infty_m}(\bar{k})$, with $m \geq 2$. Following the regularization of the mentioned unbounded contributions, effected through carrying out appropriate partial infinite summations (see § II.B), we arrive at expressions in which for instance $\mathcal{S}^{(2)}_{\sigma;\infty_2}(\bar{k})$ of our above considerations (see Eq. (128)) is replaced by the *regular* contribution to $\mathcal{S}^{(2)}_{\sigma;\infty_2}(\bar{k})$, that is $\mathcal{S}^{\mathrm{r}(2)}_{\sigma;\infty_2}(\bar{k})$, supplemented by $3[n_{0;\bar{\sigma}}/n_0 - n_{0;\sigma}/n_0](-\bar{z}/2)^{1/2}$ (see Eq. (129)) and $\mathcal{S}^{(3)}_{\sigma;\infty_2}(\bar{k})$ (see Eq. (128)) by $\mathcal{S}^{\mathrm{r}(3)}_{\sigma;\infty_2}(\bar{k})$ supplemented by $\mathcal{S}^{\mathrm{s_b}\oplus\mathrm{s}}_{\sigma;\infty_2}(\bar{k})+(3/2)\ln(-\bar{z}/r_s^3)$ (see Eq. (129)). In the concluding part of the following Section we shall very briefly discuss the consequences of these singular functions of r_s and $\bar{z}$ for the energies of the single-particle excitations.

6. An illustrative example

Here we consider in some detail the nature of the single-particle excitation energies as obtained from Eq. (105) in which $\overline{\overline{\Sigma}}_{\sigma}(\bar{k};\bar{\varepsilon})$ is replaced by the following truncated series: [79]

$$\overline{\overline{\Sigma}}_{\sigma}(\bar{k};\bar{\varepsilon}) \sim \overline{\overline{\Sigma}}_{\sigma;\infty_0}(\bar{k}) + \frac{\overline{\overline{\Sigma}}_{\sigma;\infty_1}(\bar{k})}{\bar{\varepsilon}}. \tag{145}$$

We thus have

$$\bar{\varepsilon}^{(0)}_{\bar{k}} + r_s \mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k}) + r_s^2 \frac{\mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k})}{\bar{\varepsilon}_{\bar{k};\sigma}} = \bar{\varepsilon}_{\bar{k};\sigma}. \tag{146}$$

From this we have the equivalent equations

$$x = \alpha + \frac{\beta}{x} \iff x^2 - \alpha x - \beta = 0, \tag{147}$$

where

$$x{:=}\bar{\varepsilon}_{\bar{k};\sigma},\;\; \alpha{:=}\bar{\varepsilon}^{(0)}_{\bar{k}} + r_s \mathcal{S}^{(1)}_{\sigma;\infty_0}(\bar{k}),\;\; \beta{:=}r_s^2\, \mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k}). \tag{148}$$

[79] Rather than using the expression in Eq. (121), which has its root in the series in Eq. (72), one may use the equivalent of the expression in Eq. (121) corresponding to the alternative series in Eq. (79). The normalized energy parameter $\bar{\varepsilon}_0 \equiv \varepsilon_0/e_0$ (see Eq. (103) above) in the alternative expression may be fixed either by the requirement $|\bar{\varepsilon} - \bar{\varepsilon}_0| \gg 1$, where $\bar{\varepsilon}$ is close to the expected value of the sought-after solution $\bar{\varepsilon}_{\bar{k};\sigma}$ of Eq. (105), or by the requirement that Eq. (146), with $\bar{\varepsilon}_{\bar{k};\sigma}$ in the denominator replaced by $\bar{\varepsilon}_{\bar{k};\sigma} - \bar{\varepsilon}_0$ (see Eqs. (79) and (81)) be identically satisfied by $\bar{\varepsilon} = \bar{\varepsilon}_F$ for $\bar{k} = \bar{k}_{F;\sigma} \equiv \bar{k}_{F;\bar{\sigma}}$; $\bar{\varepsilon}_F = \bar{\varepsilon}^{(0)}_F + \bar{\mu}_{\mathrm{xc}}$ can be calculated through knowledge of the total energy of the system as a function of the total number density (see footnote 78).

By *assuming* $|\beta| \ll |\alpha|$ (the "weak-coupling" limit — see above), one observes that $x \approx \alpha$, or better $x \approx \alpha + \beta/\alpha$; by iteratively continuing this procedure of refining the solution, we obtain the following infinite continued-fraction expansion (Khinchin 1964) for the solution, which we denote by x_{w} (the subscript 'w' indicates 'weak coupling'):

$$x_{\mathrm{w}} = \alpha + \frac{\beta}{\alpha+}\,\frac{\beta}{\alpha+}\,\frac{\beta}{\alpha+}\;\ldots. \tag{149}$$

If on the other hand, $|\beta| \gg |\alpha|$ (the "strong-coupling" limit; [80] we shall later discuss the appropriate sign of β in this limit), the above iteration scheme will *not* be useful as it converges towards the 'weak-coupling' solution. [81] Rather, with $f(x){:=}\alpha + \beta/x$, one should solve the equivalent problem $f^{-1}(x) = x$, where $f^{-1}(x)$ denotes the inverse of $f(x)$, defined though $f^{-1}\big(f(x)\big) \equiv f\big(f^{-1}(x)\big) = x$. With $f^{-1}(x) \equiv \beta/(x-\alpha)$, assuming, for instance, $x \approx \beta^{1/2}$ (here we are assuming $\beta > 0$; see later), [82] an iterative treatment of the latter equation yields the solution which we denote by x_{s} (the subscript 's' indicates 'strong coupling'):

$$x_{\mathrm{s}} = -\frac{\beta}{\alpha+}\,\frac{\beta}{\alpha+}\,\frac{\beta}{\alpha+}\;\ldots. \tag{150}$$

From Eqs. (149) and (150) we have $x_{\mathrm{w}} + x_{\mathrm{s}} = \alpha$.

For the quadratic equation on the RHS of Eq. (147) we have the following solutions:

$$x_{\pm}{:=}\frac{1}{2}\big\{\alpha \pm (\alpha^2 + 4\beta)^{1/2}\big\}, \tag{151}$$

[80] This "strong-coupling" limit does *not* coincide with the true 'strong-coupling' limit. This is evident from the fact that our point of departure in this Section, namely Eq. (145), is *not* the appropriate one for considerations regarding the true 'strong-coupling' regime (compare Eqs. (121) and (132)). Nonetheless, the direct implication of $|\beta| \gg |\alpha|$ for r_s (see Eq. (148)) renders identification of the latter condition with the 'strong-coupling' limit meaningful for a *finite* range of $\bar{k}$ values. To appreciate the significance of the latter statement, note that, since $\bar{\varepsilon}^{(0)}_{\bar{k}}$ is a monotonically increasing function of $\bar{k}$ (see Eq. (106)), it follows that independent of the value chosen for r_s, for a sufficiently large value of $\bar{k}$, $|\alpha|$ exceeds $|\beta|$ (see Eq. (148)), so that the "strong-coupling" limit as considered here only applies for a finite range of $\bar{k}$ values.

[81] This statement is easiest understood through a graphical representation of $\alpha+\beta/x$ in relation to line $y = x$ in the $x-y$ plane.

[82] For $|\beta| \gg |\alpha|$, the equation on the LHS of Eq. (147) can be written as $x \approx \beta/x \iff x^2 \approx \beta$, whose solution, provided $\beta > 0$, is $x \approx \beta^{1/2}$. Consistency demands that $\beta/x|_{x=\beta^{1/2}} = \beta^{1/2}$ be larger than $|\alpha|$. In other words, the "strong-coupling" solution applies so long as $\beta^{1/2} \gg |\alpha|$.

from which one indeed has $x_+ + x_- = \alpha$. It is readily verified that in fact $x_{\rm w} \equiv x_+$ and $x_{\rm s} \equiv x_-$, so that the RHS of Eq. (150) is the continued-fraction expansion (Khinchin 1964) of $\frac{1}{2}\{\alpha - (\alpha^2 + 4\beta)^{1/2}\}$.

The exact solutions to Eq. (147) reveal that in order for Eq. (147) (or Eq. (146)) to possess real solutions, it is *necessary* that $\alpha^2 \geq -4\beta$, which is satisfied in the 'weak-coupling' limit, however, its satisfaction in the 'strong-coupling' limit requires $\beta > 0$ (see above where we state that in this limit $x \approx \beta^{1/2}$ and that $\beta > 0$). We note in passing that $\alpha^2 > -4\beta$ coincides with the condition for the convergence of the continued fractions on the RHSs of Eqs. (149) and (150). With reference to our statements in the last but one paragraph of § III.E.4, we point out that our explicit calculations show the *local* contribution to $\Sigma_{\sigma;\infty_1}(k)|_{\rm s}$ to be positive (see Appendix F) so that the condition $\beta > 0$ is not ruled out (*cf.* Eqs. (187) and (F66)).

Approximating $\Sigma_\sigma(k;\varepsilon)$ by $\overline{\Sigma}_{\sigma;\infty_0}(k) + \overline{\Sigma}_{\sigma;\infty_1}(k)/\varepsilon$, from the Dyson equation for the Fourier transform of the single-particle spectral function as defined in Eq. (39) (see also Eqs. (52) and (237)) we readily obtain

$$\overline{A}_\sigma(k;\varepsilon) = \hbar\Big\{\frac{\vert\varepsilon_-\vert}{\vert\varepsilon_+ - \varepsilon_-\vert}\,\delta(\varepsilon - \varepsilon_-) + \frac{\vert\varepsilon_+\vert}{\vert\varepsilon_+ - \varepsilon_-\vert}\,\delta(\varepsilon - \varepsilon_+)\Big\}, \tag{152}$$

where (see Eqs. (148) and (103) above) $\varepsilon_\pm \equiv e_0\, x_\pm$ and where we have assumed $x_+ \neq x_-$. From Eq. (152) we obtain (*cf.* Eqs. (38) and (53))

$$\frac{1}{\hbar}\int_{-\infty}^{\infty} {\rm d}\varepsilon\; \varepsilon^{m-1}\,\overline{A}_\sigma(k;\varepsilon) = \frac{1}{\vert\varepsilon_+ - \varepsilon_-\vert}\Big\{\vert\varepsilon_-\vert\varepsilon_-^{m-1} + \vert\varepsilon_+\vert\varepsilon_+^{m-1}\Big\}. \tag{153}$$

In the 'weak-coupling' limit we have $\varepsilon_- \approx 0$ and $\varepsilon_+ \approx e_0\alpha$ when $\alpha > 0$ and $\varepsilon_- \approx e_0\alpha$ and $\varepsilon_+ \approx 0$ when $\alpha < 0$. Employing these results, from Eq. (152) we have

$$\overline{A}_\sigma(k;\varepsilon) \approx \hbar\delta(\varepsilon - e_0\alpha) \tag{154}$$

(that is, we have only one single-particle excitation whose energy is equal to $e_0\alpha$), and from Eq. (153)

$$\frac{1}{\hbar}\int_{-\infty}^{\infty} {\rm d}\varepsilon\; \varepsilon^{m-1}\,\overline{A}_\sigma(k;\varepsilon) \approx (e_0\alpha)^{m-1}, \tag{155}$$

the RHS of which exactly coincides with that of Eq. (53).

On the other hand, in the "strong-coupling" limit (see footnote 80 and note that *here* this limit is meaningful only for finite values of $\bar{k}$), $x_\pm \approx \pm\beta^{1/2}$ so that from Eq. (153) we have [83]

$$\frac{1}{\hbar}\int_{-\infty}^{\infty} {\rm d}\varepsilon\; \varepsilon^{m-1}\,\overline{A}_\sigma(k;\varepsilon) \approx \frac{1}{2}\{1 + (-1)^{m-1}\}\,\big(e_0\beta^{1/2}\big)^{m-1}, \tag{156}$$

which, with the exception of cases corresponding to *even* values of m, similar to Eq. (155) exactly reproduces the RHS of Eq. (53) for $x_\pm$. It is of significance that both Eq. (155) and Eq. (156) yield the *exact* result in Eq. (57) corresponding to $m = 1$ which concerns the interaction-independent normalization of the single-particle spectral function.

With reference to our discussions in § III.B, we point out that in general (excluding the case corresponding to $m = 1$) there is a *fundamental* difference between the moments integral in Eq. (38) (in conjunction with Eq. (37)) and moments integrals in Eqs. (53), (153), (155) and (156) which involve the Fourier transform of the single-particle spectral function. As we have indicated earlier in this paper (see also Appendix A), this follows from the fact that, for interacting systems, the Lehmann amplitudes $\{f_{s;\sigma}(\boldsymbol{r})\}$ pertaining to systems with uniform GSs are *not* single plane waves $\{\Omega^{-1/2}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})\}$, so that *non*-orthonormality that is a characteristic feature of the set of Lehmann amplitudes pertaining to *interacting* systems (see Appendix A), is *not* taken account of by Eqs. (53), (153), (155) and (156) (see our remark following Eq. (53) above). Since in the weak-coupling limit we have (symbolically) $\{f_{s;\sigma}(\boldsymbol{r})\} \approx \{\Omega^{-1/2}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})\}$ (*cf.* Eqs. (46) - (48) above), it follows that Eq. (155) (which is the equivalent of Eq. (53) in our present considerations) is a far more reliable representation of Eq. (42) (in which s' is set equal to s and E is identified with ∞) than Eq. (156) is. Although the approximate SE in Eq. (145) is undeniably too inaccurate in the strong-coupling regime (see § III.E.5 and footnote 80), it is *not* difficult to see that the deviation of Eq. (156) for even values of m from Eq. (53) (more specifically, the fact that, unlike the RHS of Eq. (53), that of Eq. (156) is *identically* vanishing for even values of m) is in reality almost entirely (insofar as small values of $\bar{k}$ are concerned; see footnote 80 and later) attributable to the severe deviation of $\{f_{s;\sigma}(\boldsymbol{r})\}$ from $\{\Omega^{-1/2}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})\}$ in the strong-coupling regime: since $\overline{A}_\sigma(k;\varepsilon)$ is positive semi-definite, it follows that for *any* $\overline{A}_\sigma(k;\varepsilon)$ which is symmetric with respect to ε (as $\overline{A}_\sigma(k;\varepsilon)$ in Eq. (152) approximately is for $\varepsilon_\pm \approx \pm e_0\beta^{1/2}$), the integrals over $(-E,E)$, $E \to \infty$, of $\varepsilon^{m-1}\,\overline{A}_\sigma(k;\varepsilon)$ must be identically vanishing for even values of m; what

[83] The principle underlying conversion of the dimensionless quantity β into one with dimension energy, namely $e_0\beta^{1/2}$, is as follows. Starting from the 'dimensionful' Dyson equation $\varepsilon_k^{(0)} + \sum_{m=0}^{\infty}\hbar\overline{\Sigma}_{\sigma;\infty_m}(k)/\varepsilon_{k;\sigma}^m = \varepsilon_{k;\sigma}$, dividing both sides by e_0, with e_0 as defined in Eq. (103), and subsequently writing $\varepsilon_{k;\sigma}^m = e_0^m(\varepsilon_{k;\sigma}/e_0)^m \equiv e_0^m\,\bar{\varepsilon}_{k;\sigma}^m$, it immediately follows that $\overline{\overline{\Sigma}}_{\sigma;\infty_m}(\bar{k}) \equiv \hbar\overline{\Sigma}_{\sigma;\infty_m}(k)/e_0^{m+1}$ (see text following Eq. (104)).

prevents this to be generally the case for the LHS of Eq. (50), with $s = s'$ (where s is justifiably identified with $\boldsymbol{k}$ in the weak-coupling regime and whence Eq. (53)), is the fact that, depending on the s, and therefore $f_{s;\sigma}(\boldsymbol{r})$, under consideration, the weight in the spectral function $\mathsf{A}_{\sigma;s,s}(\varepsilon)$, as distinct from $\overline{A}_{\sigma}(\|\boldsymbol{k}\|;\varepsilon) \equiv \overline{A}_{\sigma;\boldsymbol{k},\boldsymbol{k}}(\varepsilon)$, can be considerably asymmetrically distributed with respect to $\varepsilon = 0$; this possibility is *not* capable of being fully realized in the strong-coupling regime when the "parameter of degeneracy" α in $s = (\varsigma, \alpha) \equiv (\boldsymbol{k}, \alpha)$ (see Eq. (45) above) is *not* accounted for and s is reduced to $\boldsymbol{k}$ (see Appendix A). Concerning the insufficiency of the expression in Eq. (145) in the strong-coupling regime and its role in rendering the RHS of Eq. (156) identically vanishing for even values of m (see above where we ascribe the latter problem almost entirely to the severe deviation of $f_{s;\sigma}(\boldsymbol{r})$ from a single plane wave), we mention that a more accurate expression for the SE than that on the RHS of Eq. (145) would in essence bring about some degree of asymmetry with respect to $\varepsilon = 0$ in the corresponding $\overline{A}_{\sigma}(k;\varepsilon)$ (since the single-particle excitations with $\varepsilon_{s;\sigma} < \mu$ correspond to $(N_\sigma - 1 + N_{\bar{\sigma}})$-particle states whereas those with $\varepsilon_{s;\sigma} > \mu$ correspond to $(N_\sigma + 1 + N_{\bar{\sigma}})$-particle states; see Eq. (19) above); however, this would *not* change the fact that, in the strong-coupling regime, $\mathsf{A}_{\sigma;s,s}(\varepsilon)$ *cannot* even approximately be identified with $\overline{A}_{\sigma;\boldsymbol{k},\boldsymbol{k}}(\varepsilon)$.

The above considerations clearly show how in the weak-coupling limit, the simple asymptotic expression for the SE, as presented in Eq. (145), can reliably reproduce the exact results as presented in Eq. (53). In this connection we mention that we have performed numerical calculations within the framework of the SSDA (see Appendix C) and in doing so neglected the *non*-local contribution to $\overline{\overline{\overline{\Sigma}}}_{\sigma;\infty_1}(\bar{k})$ in Eq. (145) (*cf.* Eq. (188)); in conformity with our above theoretical findings, our calculated results for the bandwidths of ideal metals, over the entire range of the metallic densities, turn out to be qualitatively accurate and on physical grounds also quantitatively justifiable.

Now we briefly consider the cases where rather than the first two leading terms (as in Eq. (145) above), account is taken of the first $p+1$, $p \geq 2$, leading terms in the large-$|\varepsilon|$ AS for the SE (see Eq. (72) above). To keep our discussion transparent, we first restrict our considerations to the case where $\{\Sigma_{\sigma;\infty_j}(\boldsymbol{r},\boldsymbol{r}') \| j = 0, 1, \dots, p\}$ are bounded (almost everywhere) and integrable so that the employed finite-order AS (both in the coordinate and in the momentum representation) involves solely $\{1/\varepsilon^j \| j = 0, 1, \dots, p\}$ and *no* transcendental functions of ε (see § II.B — see also Eq. (128) and compare with Eq. (129)). Replacing $\overline{\Sigma}_{\sigma}(k;\varepsilon)$ in the Dyson equation (see Eq. (232) below) by the latter series, one obtains a $(p+1)$th-order polynomial equation for the single-particle energies, to be contrasted with the second-order equation in Eq. (147). The real-valuedness of the coefficients in the equation (*cf.* Eq. (148) above; see also § III.I.2 and the second paragraph of Appendix B) [84] implies that in principle this equation has $p+1$ distinct real-valued solutions (it may *in principle* also possess pairs of complex conjugate solutions, however these are pathological (see § III.D), so that provided that the constituent functions [i.e. the 'coefficients'] of the polynomial equation are calculated accurately, we expect these solutions not to occur), to be compared with the two solutions $\varepsilon_\pm$ discussed above; the contributions of *all* these solutions to the single-particle spectral function, which are poles, will be such that the integral of this function over $(-\infty, \infty)$ equals unity for *all* values of p (*cf.* Eq. (57) above or, equivalently, Eq. (38) in which m is identified with 1 and E with ∞). In the limit $p \to \infty$, these poles condense into *branch cuts* (for an explicit example see Farid (1999c, Appendix A)) and, unlike the function $\overline{A}_{\sigma}(k;\varepsilon)$ in Eq. (152) which is unbounded at the locations of the solutions of Eq. (146) (or Eq. (147)), the equivalent of this function corresponding to $p \to \infty$ is bounded almost everywhere along the real ε-axis; the pronounced peaks of this function have thus in general finite widths, which are interpreted as corresponding to the finite lifetimes of the single-particle excitations in interacting systems. Considering the fact that the *infinite*-order series for $\widetilde{G}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ in Eq. (27) and the associated *infinite*-order series for $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ are exact representations of these functions (see § III.A), we observe that by replacing the δ functions, encountered in the single-particle spectral functions pertaining to finite values of p, by Lorentzians, that is by applying the substitution

$$\delta(\varepsilon - \varepsilon_j) \rightharpoonup \frac{\eta/\pi}{(\varepsilon - \varepsilon_j)^2 + \eta^2}, \tag{157}$$

with η some appropriately chosen small positive value (decreasing for increasing values of p), an accelerated convergence towards the exact single-particle spectral function should be achieved as p is increased towards ∞. In fact, by applying such a procedure in the case corresponding to $p = 1$ which we have explicitly considered in this Section, one would view, for sufficiently small values of $|\varepsilon_+ - \varepsilon_-|$ (which condition precludes the case corresponding to the 'strong-coupling' regime where $|\varepsilon_+ - \varepsilon_-| \approx 2e_0\beta^{1/2}$ with $\beta^{1/2} \gg \alpha$), the two solutions $\varepsilon_\pm$ as representing the precursors to a single peak of finite width (of the order of $|\varepsilon_+ - \varepsilon_-|$; see Eq. (152) above) in the exact $\overline{A}_{\sigma}(k;\varepsilon)$ corresponding to $p = \infty$.

As we have seen in Eq. (118) above and shall encounter in § III.H, for some v and d, specifically for $v \equiv v_c$ and

[84] Here we neglect $\mathrm{Im}[\Sigma_\sigma(\varepsilon)]$ (see § III.I), but shall later comment on the relevance of this contribution.

$d = 3$, regularization of the unbounded contributions in $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$, which amounts to performing sums over infinite number of related unbounded terms, results in transcendental functions of z that possess both essential singularities at the point of infinity in the complex z plane (as well as at $z = 0$) *and* finite imaginary parts for $z = \varepsilon \pm i\eta$, with ε real and $\eta \downarrow 0$ (see Eqs. (113) and (114) above), and similarly for the non-integrable contributions to $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ which give rise to singular complex-valued parts in the regularized large-$|\varepsilon|$ AS for the momentum representation of the SE operator (see § III.E.3 and Appendix H). In such cases, incorporating the latter imaginary contributions while, as in the above considerations, neglecting the contributions to $\mathrm{Im}[\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)]$ which are associated with the regular, or bounded (and integrable), terms in the large-$|\varepsilon|$ AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (see § III.I) gives rise to an equation for the single-particle energies that unlike that presented in Eq. (147) is *not* real (for real ε) and polynomial, but complex and transcendental. Consequently, we expect the solutions of these equations to be complex-valued, some of which may be pathological (possessing imaginary parts with incorrect sign, arising from the approximate nature of the calculations, based on a partial incorporation of the imaginary contributions to the SE), incorrectly implying the instability of the GS of the system under consideration (see § III.D). In the present case, where the quasi-particle equations involve transcendental functions of ε (or z), the nature of solutions are not as straightforwardly classified as in the case where these equations are purely polynomial, which, following the fundamental theorem of algebra (Titchmarsh 1939, pp. 118 and 119), possess a well-specified class of solutions.

The full incorporation of the imaginary contributions of $\Sigma_\sigma(\varepsilon)$ to the large-$|\varepsilon|$ AS of this function (see § III.I) does *not* lead to any *fundamental* change in the behaviour of the corresponding single-particle excitation energies in comparison with the behaviours of those just discussed, except that it gives rise to removal of the possible pathological solutions referred to above. In general, leaving aside the contributions of the aforementioned transcendental functions of ε to the quasi-particle energies, the contribution of the regular imaginary terms may be effectively taken account of by means of a set of finite positive constants $\{\eta_j\}$ that through Eq. (157) transform the δ functions contributing to the single-particle spectral function (i.e. the one deduced through identifying *all* imaginary terms in the polynomial equation with zero) into Lorentzians. This should also apply as a means for effectively taking account of the imaginary contributions originating from the aforementioned transcendental functions of ε to the equation for the single-particle energies, provided that the real-valued solutions corresponding to the case where *all* imaginary contributions to the SE are neglected are *not* too close to the branch points of these transcendental functions (in our present considerations, these are at $z = 0$ and at the point of infinity in the complex z plane; use of Eq. (79) as the starting point of the calculations, rather than Eq. (72), changes $z = 0$ here into $z = \varepsilon_0$).

F. Evaluation of $G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$

Before proceeding with the calculation of $G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$, we explicitly specify the direction along which in the following the kinetic-energy operator $\tau(\boldsymbol{r})$ in $h_0(\boldsymbol{r})$ (see Eq. (43) above) is meant to act on functions of $\boldsymbol{r}$. In spite of the fact that $\tau(\boldsymbol{r})$ (as well as $h_0(\boldsymbol{r})$) is Hermitian in the single-particle Hilbert space of the problem at hand, this specification is *not* redundant. This follows from the fact that in our following considerations, the domain of operation of $\tau(\boldsymbol{r})$ (and of $h_0(\boldsymbol{r})$ for that matter) does *not* extend to *all* functions of $\boldsymbol{r}$ to its right, a consequence of the specific way (namely, through *local* (anti)commutation relations) in which $\tau(\boldsymbol{r})$ finds its entrance into the expressions to be considered below. In what follows, $\tau(\boldsymbol{r})$ (and $h_0(\boldsymbol{r})$) will *strictly* act on all functions of $\boldsymbol{r}$ to its right that together with $\tau(\boldsymbol{r})$ are enclosed by appropriate brackets. When wishing to indicate operation of $\tau(\boldsymbol{r})$ ($h_0(\boldsymbol{r})$) to functions of $\boldsymbol{r}$ to its left, we employ the notation $\tau^+(\boldsymbol{r})$ ($h_0^+(\boldsymbol{r})$), with the pertinent functions of $\boldsymbol{r}$ enclosed by the same brackets that enclose $\tau^+(\boldsymbol{r})$ ($h^+(\boldsymbol{r})$).

Using the canonical anticommutation relations in Eq. (29), we deduce

$$\widehat{A}_\sigma(\boldsymbol{r}) := \big[\hat{\psi}_\sigma(\boldsymbol{r}), \widehat{H}\big]_- = \big\{\hat{\alpha}(\boldsymbol{r})\,\hat{\psi}_\sigma(\boldsymbol{r})\big\}, \tag{158}$$

where

$$\hat{\alpha}(\boldsymbol{r}) := h_0(\boldsymbol{r}) + \sum_{\sigma'} \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}'')\hat{\psi}_{\sigma'}(\boldsymbol{r}''). \tag{159}$$

By enclosing the RHS of Eq. (158) within curly brackets, we have made explicit the fact that $h_0(\boldsymbol{r})$ that features in the defining expression for $\hat{\alpha}(\boldsymbol{r})$ in Eq. (159), acts *solely* upon $\hat{\psi}_\sigma(\boldsymbol{r})$ and *no* other function to the right of the enclosed function (see above). Since $\widehat{H}$ is Hermitian, by Hermitian conjugation of Eq. (158) we obtain

$$\widehat{A}^\dagger_\sigma(\boldsymbol{r}) \equiv -\big[\hat{\psi}^\dagger_\sigma(\boldsymbol{r}), \widehat{H}\big]_- = \{\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\,\hat{\alpha}^\dagger(\boldsymbol{r})\}, \tag{160}$$

where $\hat{\alpha}^\dagger(\boldsymbol{r})$, according to Eq. (159), involves $h_0^+(\boldsymbol{r})$ and thus $\tau^+(\boldsymbol{r})$ which operates solely on $\hat{\psi}^\dagger_\sigma(\boldsymbol{r})$ to its left, so that we have $\{\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\tau^+(\boldsymbol{r})\} \equiv \{\tau(\boldsymbol{r})\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\}$. We should emphasize that, although our detailed specification of $\widehat{A}_\sigma(\boldsymbol{r})$ and of its Hermitian conjugate (as reflected in our introduction of curly braces in Eqs. (158) and (160)) seems excessive at this stage (and it is admittedly so as far as evaluation of $G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ is concerned), such a specification is of *vital* significance for the correct determination of $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, when $m > 2$. Further, our experience shows that without appropriate structuring of various contributions, as achieved through introducing $\widehat{A}_\sigma(\boldsymbol{r})$, the explosive proliferation of terms with their various indices and arguments renders determination of the expression for $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, with $m \geq 4$, well nigh impossible.

From Eqs. (34) and (158) it follows that

$$G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') = \hbar\langle\Psi_{N;0}|[\widehat{A}_\sigma(\boldsymbol{r}),\hat{\psi}_\sigma^\dagger(\boldsymbol{r}')]_+|\Psi_{N;0}\rangle. \quad (161)$$

Making use of the result on the RHS of Eq. (159) and the anticommutation relations in Eq. (29), we arrive at [85]

$$G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') = \hbar\Big\{\big[h_0(\boldsymbol{r})+v_H(\boldsymbol{r};[n])\big]\delta(\boldsymbol{r}-\boldsymbol{r}') - v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\Big\}, \quad (162)$$

where the Hartree potential $v_H(\boldsymbol{r};[n])$ is defined in Eq. (14) above, in which the *total* number density n is defined through (see Eq. (K1))

$$n(\boldsymbol{r}) \equiv n_\sigma(\boldsymbol{r}) + n_{\bar{\sigma}}(\boldsymbol{r}) \equiv \sum_{\sigma'}\langle\Psi_{N;0}|\hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r})\hat{\psi}_{\sigma'}(\boldsymbol{r})|\Psi_{N;0}\rangle; \quad (163)$$

since our considerations are *not* restricted to systems of spin-1/2 fermions, we have the general expression

$$n_{\bar{\sigma}}(\boldsymbol{r}) \equiv \sum_{\sigma'\neq\sigma} n_{\sigma'}(\boldsymbol{r}), \quad (164)$$

where the summation is over 2s contributions (*cf.* Eq. (21) above). Further, in Eq. (162),

$$\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) := \langle\Psi_{N;0}|\hat{\psi}_\sigma^\dagger(\boldsymbol{r}')\hat{\psi}_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle \quad (165)$$

stands for the GS partial density matrix pertaining to the interacting system; in our present work, it is real and symmetric (see Appendix B). The non-orthonormality of the set $\{f_{s;\sigma}(\boldsymbol{r})\}$ pertaining to interacting systems (see Appendix A) implies that $\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}')$ is *strictly* non-idempotent, that is

$$\int \mathrm{d}^d r''\; \varrho_\sigma(\boldsymbol{r},\boldsymbol{r}'')\,\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r}') \not\equiv \varrho_\sigma(\boldsymbol{r},\boldsymbol{r}'). \quad (166)$$

In the case of $v \equiv v_c$ in $d = 3$, the sum $h_0(\boldsymbol{r}) + v_H(\boldsymbol{r};[n])$ on the RHS of Eq. (162) is identical with $\tau(\boldsymbol{r}) + u(\boldsymbol{r}) + v_H(\boldsymbol{r};[n'])$, independent of ϖ_κ, so that it is well-defined for $\kappa \downarrow 0$ (see § II.A and Eqs. (11) and (15)).

For completeness, through making use of the completeness relation

$$\sum_{M_\sigma,M_{\bar{\sigma}},s} |\Psi_{M_\sigma,M_{\bar{\sigma}};s}\rangle\langle\Psi_{M_\sigma,M_{\bar{\sigma}};s}| = \mathcal{I}, \quad (167)$$

where $\mathcal{I}$ stands for the unit operator in the Fock space, taking into account the orthogonality of the eigenstates of $\{\widehat{N}_\sigma\}$ corresponding to different eigenvalues, we obtain the familiar expression

$$\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}') = \sum_s^{<} f_{s;\sigma}^*(\boldsymbol{r}) f_{s;\sigma}(\boldsymbol{r}'). \quad (168)$$

Here $\sum_s^<$ denotes the sum over all s corresponding to $\varepsilon_{s;\sigma} < \mu$. This specification is necessary through our use of functions from the set $\{f_{s;\sigma}(\boldsymbol{r})\}$ (see Eq. (18) above) which encompasses two fundamentally distinct classes of functions, [86] namely those corresponding to $\varepsilon_{s;\sigma} < \mu$ and those corresponding to $\varepsilon_{s;\sigma} > \mu$; had we not employed symbols $f_{s;\sigma}^*(\boldsymbol{r})$ and $f_{s;\sigma}(\boldsymbol{r}')$, but instead $\langle\Psi_{N;0}|\hat{\psi}_\sigma^\dagger(\boldsymbol{r})|\Psi_{N_\sigma-1,N_{\bar{\sigma}};s}\rangle$ and $\langle\Psi_{N_\sigma-1,N_{\bar{\sigma}};s}|\hat{\psi}_\sigma(\boldsymbol{r}')|\Psi_{N;0}\rangle$, respectively, the 'symbolic' restriction, as implied by $<$ in $\sum_s^<$, would *not* have been necessary. It is important to appreciate the significance of these aspects, since in spite of the *restriction* that is implied by $<$ in $\sum_s^<$ (and similarly by $>$ in $\sum_s^>$, denoting a sum over all s corresponding to $\varepsilon_{s;\sigma} > \mu$), nonetheless Eq. (31) applies. In view of these statements, it is interesting to consider the similar expression as in Eq. (168) for the Slater-Fock density matrix pertaining to the 'non-interacting' Hamiltonian $\widehat{H}_0$ in Eq. (54). With reference to the eigenvalue problem in Eq. (56) we have

$$\varrho_{\mathrm{s};\sigma}(\boldsymbol{r},\boldsymbol{r}') = \sum_\varsigma^{<} \varphi_{\varsigma;\sigma}^*(\boldsymbol{r})\varphi_{\varsigma;\sigma}(\boldsymbol{r}'), \quad (169)$$

which in view of the expression in Eq. (46) and the succeeding text (see also the text following Eq. (56) above) indeed corresponds to $\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (168) for $v \to 0$. In Eq. (169), $\sum_\varsigma^<$ denotes a sum over all ς corresponding to $\varepsilon_{\varsigma;\sigma}^{(0)} < \mu^{(0)}$ (see Eq. (168) above and the subsequent text), where $\mu^{(0)}$ stands for the 'chemical potential' of the 'non-interacting' N-particle system. Taking into account the normalization to unity of the single-particle wavefunctions $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$, making use of $\varrho_{\mathrm{s};\sigma}(\boldsymbol{r},\boldsymbol{r}) \equiv n_{0;\sigma}(\boldsymbol{r})$ and $\int \mathrm{d}^d r\; n_{0;\sigma}(\boldsymbol{r}) = N_\sigma$, from Eq. (169) it follows that

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[85] As we have indicated earlier (see § III.A), $G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ is a c-number, so that $\nabla_{\boldsymbol{r}}^2$ involved in $h_0(\boldsymbol{r})$ (see Eq. (43) above) on the RHS of Eq. (162) solely operates on $\delta(\boldsymbol{r}-\boldsymbol{r}')$ to its right and on *no* function outside the curly brackets.

[86] Another way of stating this fact is that the compound variable s corresponding to cases $\varepsilon_{s;\sigma} < \mu$ is inherently different from that corresponding to $\varepsilon_{s;\sigma} > \mu$.

$$\sum_{\varsigma} \Theta\big(\mu^{(0)} - \varepsilon^{(0)}_{\varsigma;\sigma}\big) = N_\sigma; \tag{170}$$

that is the number of terms involved in the summation on the RHS of Eq. (169) is *exactly* equal to N_σ. This is in stark contrast with the number of terms involved in the summation on the RHS of Eq. (168) which, under the condition that $N_\sigma \neq 0$, is *infinitely large* (as evidenced by the completeness relation in Eq. (31)), [87] even though naturally $\int \mathrm{d}^d r\; \varrho_\sigma(\boldsymbol{r},\boldsymbol{r}) = N_\sigma$ holds (see our considerations leading to Eqs. (48) and (50) in § III.B). Such a distinctive contrast between $\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and $\varrho_{\mathrm{s};\sigma}(\boldsymbol{r},\boldsymbol{r}')$ reveals one of the most dramatic consequences of interaction and thereby of the *overcompleteness* of the set of the Lehmann amplitudes $\{f_{s;\sigma}(\boldsymbol{r})\}$ (see Appendix A).

The expression for $G_{0;\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ is readily deduced from that in Eq. (162) through setting the coupling constant of the particle-particle interaction to zero and noting that, in $\widehat{H}_0$, the external potential $u(\boldsymbol{r})$ is replaced by $u(\boldsymbol{r}) + w_\sigma(\boldsymbol{r})$ (*cf.* Eqs. (55) and (62)); thus one obtains

$$G_{0;\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') = \hbar\Big\{ \big[h_0(\boldsymbol{r}) + w_\sigma(\boldsymbol{r})\big]\delta(\boldsymbol{r}-\boldsymbol{r}')\Big\}, \tag{171}$$

which similar to $G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (162) is a *c*-number. As in Eq. (162), we have emphasized this fact by means of curly brackets on the RHS of Eq. (171); in the following we shall *not* employ this convention when there is no likelihood for confusion.

Before closing this Section, it is relevant to point out that, although in the case of when $v \equiv v_c$ we need to effect the transformation in Eq. (11), which through Eq. (43) results in the corresponding $h_0(\boldsymbol{r})$ undergoing the transformation (see Eq. (5))

$$h_0(\boldsymbol{r}) \rightharpoonup h_0(\boldsymbol{r}) - \varpi_\kappa, \tag{172}$$

such a transformation must *not* be effected insofar as the $h_0(\boldsymbol{r})$ in Eq. (171) is concerned. This follows from the fact that ϖ_κ, which according to Eq. (5) is proportional to the coupling constant of the particle-particle interaction (i.e., e^2), is identically vanishing for the *non*-interacting system.

1. Evaluation of $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')$

From Eqs. (73), (76), (162) and (171) we obtain

$$\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{\hbar}\Big\{ v_H(\boldsymbol{r};[n])\delta(\boldsymbol{r}-\boldsymbol{r}') - v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\Big\} \equiv \Sigma^{\mathrm{HF}}(\boldsymbol{r},\boldsymbol{r}';[\varrho_\sigma]), \tag{173}$$

where $\Sigma^{\mathrm{HF}}(\boldsymbol{r},\boldsymbol{r}';[\varrho_\sigma])$ stands for the non-local SE within the Hartree-Fock framework. Clearly, $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')$ does not *explicitly* depend on the single-particle spin index σ. We point out, however, that this SE involves both the *exact* number density n and the *exact* single-particle density matrix ϱ_σ, so that $\Sigma^{\mathrm{HF}}(\boldsymbol{r},\boldsymbol{r}';[\varrho_\sigma])$ should be distinguished from that which is determined within the self-consistent Hartree-Fock framework where ϱ_σ is replaced by the Slater-Fock density matrix $\varrho_{\mathrm{s};\sigma}$.

2. The case of Coulomb-interacting fermions in the thermodynamic limit

In the case where $v \equiv v_c$, $v_H(\boldsymbol{r};[n])$ on the RHS of Eq. (173) must be replaced by $v_H(\boldsymbol{r};[n'])$ (see Eq. (15) above). This follows from the fact that, as we have pointed out in the closing part of the previous Section, in this case $h_0(\boldsymbol{r})$ in Eq. (171) must *not* be subjected to the transformation in Eq. (172) so that $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')$ 'inherits' $v_H(\boldsymbol{r};[n'])$ from the expression for $G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (162) (see our remark in the paragraph directly following Eq. (171) above). We thus have

$$\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{\hbar}\Big\{ v_H(\boldsymbol{r};[n'])\delta(\boldsymbol{r}-\boldsymbol{r}') - v_c(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\Big\}. \tag{174}$$

G. Evaluation of $G_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')$

Making use of Eq. (158), while employing the definition in Eq. (34), we have

$$G_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}') = \hbar\langle\Psi_{N;0}|\Big[\big[\widehat{A}_\sigma(\boldsymbol{r}),\widehat{H}\big]_-,\hat{\psi}^\dagger_\sigma(\boldsymbol{r}')\Big]_+|\Psi_{N;0}\rangle. \tag{175}$$

As we have indicated earlier, direct evaluation of the anticommutator and subsequently the commutator in this expression leads to a vast number of terms and therefore should not be attempted. On the other hand, by employing the identity

$$\begin{aligned}\Big[\big[\widehat{A}_\sigma(\boldsymbol{r}),\widehat{H}\big]_-,\hat{\psi}^\dagger_\sigma(\boldsymbol{r}')\Big]_+ &\equiv \widehat{A}_\sigma(\boldsymbol{r})\big[\widehat{H},\hat{\psi}^\dagger_\sigma(\boldsymbol{r}')\big]_- \\ &+\widehat{A}_\sigma(\boldsymbol{r})\hat{\psi}^\dagger_\sigma(\boldsymbol{r}')\widehat{H} - \widehat{H}\widehat{A}_\sigma(\boldsymbol{r})\psi^\dagger_\sigma(\boldsymbol{r}') \\ &+\hat{\psi}^\dagger_\sigma(\boldsymbol{r}')\widehat{A}_\sigma(\boldsymbol{r})\widehat{H} - \big[\hat{\psi}^\dagger_\sigma(\boldsymbol{r}'),\widehat{H}\big]_-\widehat{A}_\sigma(\boldsymbol{r}) \\ &-\widehat{H}\hat{\psi}^\dagger_\sigma(\boldsymbol{r}')\widehat{A}_\sigma(\boldsymbol{r}),\end{aligned} \tag{176}$$

one achieves considerable simplification by the fact that in calculating $G_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')$ according to the expression

[87] This fact underlies the property that, for systems in the thermodynamic limit, $\mu^{\mp}_{N;\sigma}$ (see Eq. (23)) are *accumulation* points of the set of single-particle excitations in these systems; correspondingly, $z = \mu^{\mp}_{N;\sigma}$ are singular points of both $\widetilde{G}_\sigma(z)$ and $\widetilde{\Sigma}_\sigma(z)$ (Farid 1999a,c). Note that, for metallic systems, $\mu^{-}_{N;\sigma} \equiv \varepsilon_F$ (independent of σ so long as $N_\sigma \neq 0$). See footnote 2.

in Eq. (175), $\widehat{H}$ in the second, third, fourth and sixth terms on the RHS of Eq. (176) can be replaced by the c-number $E_{N;0}$. Moreover, the commutation of $\widehat{H}$ with $\hat{\psi}_\sigma^\dagger(\boldsymbol{r}')$, which according to Eq. (160) is equal to $\widehat{A}_\sigma^\dagger(\boldsymbol{r}')$, results in the desirable situation in which in comparison with $\widehat{H}$, the number of field operators is decreased by one (see Eqs. (158) and (159)). Making use of the result in Eq. (176), from Eq. (175) one readily obtains (*cf.* Eq. (34) in which m is identified with 1)

$$G_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}') = \hbar\langle\Psi_{N;0}|\big[\widehat{A}_\sigma(\boldsymbol{r}),\widehat{A}_\sigma^\dagger(\boldsymbol{r}')\big]_+|\Psi_{N;0}\rangle. \quad (177)$$

This expression makes explicit the *general* property $G_{\sigma;\infty_m}(\boldsymbol{r}',\boldsymbol{r}) \equiv G_{\sigma;\infty_m}^*(\boldsymbol{r},\boldsymbol{r}')$; since in this work we choose the GS wavefunction to be real valued, we have, however, $G_{\sigma;\infty_m}^*(\boldsymbol{r},\boldsymbol{r}') \equiv G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ (see Appendix B) so that

$$G_{\sigma;\infty_m}(\boldsymbol{r}',\boldsymbol{r}) \equiv G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'),\;\; \forall\, m. \quad (178)$$

Despite the validity of this symmetry property for *all* m, it turns out that only for *odd* values of m, use of identities similar to that in Eq. (176) results in an *explicitly* symmetric $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ (see footnote 45).

Making use of the expression for $\widehat{A}_\sigma(\boldsymbol{r})$ in Eq. (158) and the anticommutation relations in Eq. (29) followed by a process of normal-ordering of the field operators, we arrive at

$$\begin{aligned} G_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}') = \hbar\Big\{ \Big[& h_0(\boldsymbol{r})h_0(\boldsymbol{r}') \\ & + h_0(\boldsymbol{r})v_H(\boldsymbol{r}';[n]) + h_0(\boldsymbol{r}')v_H(\boldsymbol{r};[n]) \\ & + \mathcal{A}(\boldsymbol{r},\boldsymbol{r}) + \int \mathrm{d}^d r''\; v^2(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')\Big]\,\delta(\boldsymbol{r}-\boldsymbol{r}') \\ & - \big(h_0(\boldsymbol{r})+h_0(\boldsymbol{r}')\big)v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \\ & - v^2(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \\ & + v(\boldsymbol{r}-\boldsymbol{r}')\big(\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')+\mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big)\Big\}, \end{aligned} \quad (179)$$

where the functions $\mathcal{A}(\boldsymbol{r},\boldsymbol{r}')$ and $\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ are defined in Appendix B (see Eqs. (B28) and (B29) respectively). We note in passing that $\mathcal{A}(\boldsymbol{r}',\boldsymbol{r}) \equiv \mathcal{A}(\boldsymbol{r},\boldsymbol{r}')$, but $\mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r}) \not\equiv \mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')$, and further that

$$\begin{aligned} & E_{N;0} \equiv \langle\Psi_{N;0}|\widehat{H}|\Psi_{N;0}\rangle \\ & = \sum_\sigma \int \mathrm{d}^d r\; \{\lim_{\boldsymbol{r}'\to\boldsymbol{r}} h_0(\boldsymbol{r})\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) - \frac{1}{2}\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r})\}, \end{aligned} \quad (180)$$

where the limit $\boldsymbol{r}'\to\boldsymbol{r}$ is necessary owing to $\nabla_{\boldsymbol{r}}^2$ in the definition for $h_0(\boldsymbol{r})$ (see Eq. (43) above). Making use of the fact that

$$\begin{aligned} -\frac{1}{2}\int \mathrm{d}^d r\; \sum_\sigma \mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}) \equiv \frac{N(N-1)}{2}\int \mathrm{d}^d r \\ \times \int \mathrm{d}^d r'\; v(\boldsymbol{r}-\boldsymbol{r}')\sum_{\sigma,\sigma'} g_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}'), \end{aligned} \quad (181)$$

with $g_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}')$ the van Hove pair-correlation function (see Eqs. (B17) and (F103)), the expression in Eq. (180) transforms into the standard expression for $E_{N;0}$ (for example March, *et al.* (1967, p. 10)). In the thermodynamic limit we have $N(N-1)\,g_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}') = n_0^2\,\mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}')$, where n_0 is the total concentration of the fermions (see Eq. (9) above) and $\mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}')$ the *normalized* van Hove pair-correlation function (see Eq. (B20)). We note in passing that following Galitskii and Migdal (1958) we have $E_{N;0} = \hbar^{-1}\int \mathrm{d}^d r\; \lim_{\boldsymbol{r}'\to\boldsymbol{r}} \int_{-\infty}^{\mu} \mathrm{d}\varepsilon\; [\varepsilon + h_0(\boldsymbol{r})]\sum_\sigma A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (see Eqs. (22), (39) and (43) above).

The expression for $G_{0;\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')$ is readily obtained from Eq. (179) through equating the coupling constant of the particle-particle interaction in Eq. (179) with zero and replacing h_0 herein by $h_{0;\sigma} \equiv h_0 + w_\sigma$ defined in Eq. (55) above. Thus,

$$G_{0;\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}') = \hbar\, h_{0;\sigma}(\boldsymbol{r})h_{0;\sigma}(\boldsymbol{r}')\,\delta(\boldsymbol{r}-\boldsymbol{r}'). \quad (182)$$

1. Evaluation of $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$

From the expression in Eq. (83), making use of the result in Eq. (162), one readily obtains (see Eq. (77) above)

$$\begin{aligned} \langle\boldsymbol{r}|G_{\sigma;\infty_2}^2|\boldsymbol{r}'\rangle = \hbar^2\Big\{ & \Big[\big(h_0(\boldsymbol{r})+v_H(\boldsymbol{r};[n])\big) \\ & \times\big(h_0(\boldsymbol{r}')+v_H(\boldsymbol{r}';[n])\big)\Big]\delta(\boldsymbol{r}-\boldsymbol{r}') \\ & - \Big[h_0(\boldsymbol{r})+h_0(\boldsymbol{r}')+v_H(\boldsymbol{r};[n])+v_H(\boldsymbol{r}';[n])\Big] \\ & \times v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \\ & + \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r})\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}'')v(\boldsymbol{r}''-\boldsymbol{r}')\Big\}. \end{aligned} \quad (183)$$

From this one immediately deduces that

$$\langle\boldsymbol{r}|G_{0;\sigma;\infty_2}^2|\boldsymbol{r}'\rangle = \hbar^2 h_{0;\sigma}(\boldsymbol{r})h_{0;\sigma}(\boldsymbol{r}')\,\delta(\boldsymbol{r}-\boldsymbol{r}'). \quad (184)$$

It follows that $\hbar^{-3}G_{0;\sigma;\infty_2}$ and $\hbar^{-2}G_{0;\sigma;\infty_3}$ in the expression for $\Sigma_{\sigma;\infty_1}$ in Eq. (74) exactly cancel, leading to the expected result that $\Sigma_{\sigma;\infty_m}$ must *not* depend on w_σ for $m \geq 1$ (see the text following Eqs. (75) and (76)). From Eqs. (74) (or Eq. (77)), (179), (182), (183) and (184) we eventually obtain

$$\begin{aligned} \Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{\hbar}\Big\{ & \Big[\mathcal{A}(\boldsymbol{r},\boldsymbol{r}) - v_H^2(\boldsymbol{r};[n]) \\ & + \int \mathrm{d}^d r''\; v^2(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')\Big]\delta(\boldsymbol{r}-\boldsymbol{r}') \\ & - v^2(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \\ & + v(\boldsymbol{r}-\boldsymbol{r}')\big[\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')+\mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big] \\ & + \big[v_H(\boldsymbol{r};[n])+v_H(\boldsymbol{r}';[n])\big]v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \\ & - \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r}')\Big\}. \end{aligned} \quad (185)$$

It is interesting to note that similar to $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')$, $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ consists of both *local* and *non-local* contributions and that, analogous to $\Sigma_{\sigma;\infty_0}$ (see Eq. (173)), *only* the non-local contribution to $\Sigma_{\sigma;\infty_1}$ *explicitly* depends on the spin index σ. This aspect directly exposes the significance of *non*-local contributions to the SE operator in representing the *direct* influence of the spin state of a single-particle excitation on its behaviour. This result in addition unequivocally demonstrates that the SE operator necessarily *explicitly* depends on σ, and further that any *local* approximation to the ε-dependent part of $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ neglects this explicit dependence at least to order $1/\varepsilon$ for large $|\varepsilon|$; in fact, our considerations in §§ III.H.1,2 establish that unless $v \equiv v_c$ (and in this case, unless $n_\sigma(\boldsymbol{r}) \not\equiv n_{\bar{\sigma}}(\boldsymbol{r})$), the local part of $\Sigma_{\sigma;\infty_2}$ is also explicitly *independent* of σ and the explicit dependence on σ of $\Sigma_{\sigma;\infty_2}$ is associated with its non-local part. [88] Our considerations in § III.H.2 reveal that some explicitly σ-dependent terms in $\Sigma_{\sigma;\infty_2}$, which ordinarily are *non-local*, transmute into *local* contributions as $v \rightharpoonup v_c$, $d \rightharpoonup 3$, so that for the Coulomb-interacting fermions in $d=3$, also the local contribution to $\Sigma_{\sigma;\infty_2}$ *explicitly* depends on σ. Consequently, a *local* approximation to the ε-dependent part of $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ that may prove reliable (for a certain range of ε) in applications corresponding to short-range and bounded v, should necessarily be less satisfactory for $v \equiv v_c$ in $d=3$.

2. *The case of Coulomb-interacting fermions in the thermodynamic limit*

We now exclusively discuss the case of systems of fermions interacting through v_c in $d=3$. One immediately observes that the expression in Eq. (185) is *not* directly amenable to explicit (numerical) calculation, for in this case several of the terms contain unbounded contributions for $\kappa \downarrow 0$. We shall now present a re-formulation of the expression in Eq. (185) which is free from such contributions.

In Appendix F we show that, although the individual terms on the RHS of Eq. (185) enclosed by square brackets and post-multiplied by $\delta(\boldsymbol{r}-\boldsymbol{r}')$ are unbounded for the case $v \equiv v_c$ and $d=3$, their *total* contribution, namely (see Eq. (F2))

$$\mathcal{A}'(\boldsymbol{r},\boldsymbol{r}) := \mathcal{A}(\boldsymbol{r},\boldsymbol{r}) - v_H^2(\boldsymbol{r};[n]) + \int \mathrm{d}^d r''\, v^2(\boldsymbol{r}-\boldsymbol{r}'') n(\boldsymbol{r}''), \tag{186}$$

is a bounded function for this case. Thus, for the *local* part of $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ we have the well-defined expression

$$\Sigma^{\mathrm{l}}_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{\hbar}\mathcal{A}'(\boldsymbol{r},\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{187}$$

In a similar manner, making use of Eqs. (F110) and (F113), for the *non*-local part of $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ we obtain

$$\begin{aligned}\Sigma^{\mathrm{nl}}_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{\hbar}\Big\{ &-v^2(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \\ &+v(\boldsymbol{r}-\boldsymbol{r}')\big[\mathcal{B}''_\sigma(\boldsymbol{r},\boldsymbol{r}') + \mathcal{B}''_\sigma(\boldsymbol{r}',\boldsymbol{r})\big] \\ &-\int \mathrm{d}^d r''\, v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'') \\ &\qquad\times \varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r})\Big\},\end{aligned} \tag{188}$$

where we have defined $\mathcal{B}''_\sigma$ in Eq. (F113). We point out that our use of d and v here (as opposed to $d=3$ and $v \equiv v_c$) is meant to convey the fact that the results in Eqs. (186) and (188) are general and *not* specific to $d=3$ and $v \equiv v_c$.

As can be immediately observed, the individual contributions on the RHS of Eq. (188) are *not* bounded for $v \equiv v_c$ in $d=3$ as $\|\boldsymbol{r}-\boldsymbol{r}'\| \to 0$, the most singular contribution being the first term, which for $\|\boldsymbol{r}-\boldsymbol{r}'\| \to 0$ diverges like $1/\|\boldsymbol{r}-\boldsymbol{r}'\|^2$ (in this limit, $\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \to n_\sigma(\boldsymbol{r})$). This divergence is integrable in $d=3$, so that $\Sigma^{\mathrm{nl}}_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ can be Fourier transformed with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$ (see conditions (B) and (C) in § II.B). As we shall see in § III.H.1, $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ involves the contribution $-\hbar^{-1}v^3(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$ (see Eq. (212) below) which for $v \equiv v_c$ in $d=3$ is *not* integrable. We shall however show (see Appendix H) that a re-summation of the infinite series of functions $-v_c^m(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})/z^{m-1}$, $m \ge 3$, each of which is non-integrable (see condition (B) in § II.B) for $m \ge 3$, gives rise to an integrable contribution which is amenable to Fourier transformation (for some relevant details see § II.B).

H. Evaluation of $G_{\sigma;\infty_4}(\boldsymbol{r},\boldsymbol{r}')$

From Eq. (34), along the lines of § III.F we obtain

$$G_{\sigma;\infty_4}(\boldsymbol{r},\boldsymbol{r}') = \hbar\langle\Psi_{N;0}|\big[\widehat{L}\widehat{A}_\sigma(\boldsymbol{r}), \widehat{A}^\dagger_\sigma(\boldsymbol{r}')\big]_+|\Psi_{N;0}\rangle. \tag{189}$$

It is interesting to compare $G_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ and $G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ in Eqs. (30) and (161), on the one hand, and $G_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')$ and $G_{\sigma;\infty_4}(\boldsymbol{r},\boldsymbol{r}')$ in Eqs. (177) and (189), on the other hand, from which one observes that, in the case of the latter two functions (to be precise, *distributions*), the operators $\widehat{A}_\sigma(\boldsymbol{r})$ and $\widehat{A}^\dagger_\sigma(\boldsymbol{r}')$ have taken over the role played by $\hat{\psi}_\sigma(\boldsymbol{r})$ and $\hat{\psi}^\dagger_\sigma(\boldsymbol{r}')$, respectively. This similarity obtains for *all* pairs $G_{\sigma;\infty_{2m-1}}(\boldsymbol{r},\boldsymbol{r}')$ and $G_{\sigma;\infty_{2m}}(\boldsymbol{r},\boldsymbol{r}')$, $m \ge 1$ where, at each level, new operators replace those

[88] Thus, leaving aside the case corresponding to $v \equiv v_c$, any approximation to $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, the local part of whose ε-dependent term to second order in $1/\varepsilon$ *explicitly* depends on σ, is necessarily erroneous.

at lower levels of the hierarchy (analogous to $\widehat{A}_\sigma(\boldsymbol{r})$ replacing $\hat{\psi}_\sigma(\boldsymbol{r})$). It should, however, be noted that, contrary to $\hat{\psi}_\sigma(\boldsymbol{r})$ and $\hat{\psi}_\sigma^\dagger(\boldsymbol{r}')$, the subsequent operators are *not* canonical, that is they do *not* satisfy the set of anticommutation relations as given in Eq. (29).

By some straightforward algebra, the expression in Eq. (189) can be rearranged into the following form:

$$G_{\sigma;\infty_4}(\boldsymbol{r},\boldsymbol{r}') = h_0(\boldsymbol{r}')\, G_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}') + \hbar \sum_{\sigma'} \int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'') \times \langle \Psi_{N;0}| \Big[\big[\hat{A}_\sigma(\boldsymbol{r}), \widehat{H}\big]_-, \hat{\xi}_{\sigma,\sigma'}(\boldsymbol{r}',\boldsymbol{r}'') \Big]_+ |\Psi_{N;0}\rangle, \quad (190)$$

where

$$\hat{\xi}_{\sigma,\sigma'}(\boldsymbol{r}',\boldsymbol{r}'') := \hat{\psi}_\sigma^\dagger(\boldsymbol{r}')\hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r}'')\hat{\psi}_{\sigma'}(\boldsymbol{r}''). \quad (191)$$

A detailed investigation reveals that it is technically advantageous to employ the following identity for the purpose of further simplifying the result in Eq. (190),

$$\langle \Psi_{N;0}| \Big[\big[\hat{A}_\sigma, \widehat{H}\big]_-, \hat{\xi}_{\sigma,\sigma'} \Big]_+ |\Psi_{N;0}\rangle = \langle \Psi_{N;0}| \Big[\big[\widehat{H}, \hat{\xi}_{\sigma,\sigma'}\big]_-, \hat{A}_\sigma \Big]_+ |\Psi_{N;0}\rangle. \quad (192)$$

After some algebra, we obtain

$$\begin{aligned}\big[\widehat{H}, \hat{\xi}_{\sigma,\sigma'}(\boldsymbol{r}',\boldsymbol{r}'')\big]_- &= h_0(\boldsymbol{r}')\, \hat{\xi}_{\sigma,\sigma'}(\boldsymbol{r}',\boldsymbol{r}'') \\ &+ \lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''} \tau(\boldsymbol{r}'') \big[\hat{\psi}_\sigma^\dagger(\boldsymbol{r}')\hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r}'')\hat{\psi}_{\sigma'}(\tilde{\boldsymbol{r}}'') - \hat{\psi}_\sigma^\dagger(\boldsymbol{r}')\hat{\psi}_{\sigma'}^\dagger(\tilde{\boldsymbol{r}}'')\hat{\psi}_{\sigma'}(\boldsymbol{r}'')\big] \\ &+ v(\boldsymbol{r}'-\boldsymbol{r}'')\, \hat{\psi}_\sigma^\dagger(\boldsymbol{r}')\hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r}'')\hat{\psi}_{\sigma'}(\boldsymbol{r}'') \\ &+ \sum_{\sigma_1'} \int \mathrm{d}^d r_1''\; v(\boldsymbol{r}'-\boldsymbol{r}_1'') \\ &\quad\times \hat{\psi}_\sigma^\dagger(\boldsymbol{r}')\hat{\psi}_{\sigma_1'}^\dagger(\boldsymbol{r}_1'')\hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r}'')\hat{\psi}_{\sigma'}(\boldsymbol{r}'')\hat{\psi}_{\sigma_1'}(\boldsymbol{r}_1''). \end{aligned} \quad (193)$$

In evaluating the anticommutation of $\big[\widehat{H}, \hat{\xi}_{\sigma,\sigma'}\big]_-$ with $\hat{A}_\sigma$, we make use of the expression in Eq. (158). After some lengthy but otherwise straightforward algebra, we arrive at

$$\begin{aligned} G_{\sigma;\infty_4}(\boldsymbol{r},\boldsymbol{r}') = \hbar \Big\{ \Big[& h_0(\boldsymbol{r})h_0(\boldsymbol{r})h_0(\boldsymbol{r}) \\ &+ \big\{h_0(\boldsymbol{r})h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}')h_0(\boldsymbol{r}') + h_0(\boldsymbol{r})h_0(\boldsymbol{r}')\big\}\, v_H(\boldsymbol{r};[n]) \\ &+ \big\{\mathcal{A}(\boldsymbol{r},\boldsymbol{r})h_0(\boldsymbol{r}') + \mathcal{A}(\boldsymbol{r}',\boldsymbol{r}')h_0(\boldsymbol{r}) + \mathcal{A}(\boldsymbol{r},\boldsymbol{r}')h_0(\boldsymbol{r})\big\} \\ &+ \int \mathrm{d}^d r''\; \big\{v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'') + v(\boldsymbol{r}'-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\big\}\, n(\boldsymbol{r}'')\, h_0(\boldsymbol{r}) \\ &+ \int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')\, h_0(\boldsymbol{r}') \\ &+ \int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'') \lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''} \tau(\boldsymbol{r}'')\, v(\boldsymbol{r}-\boldsymbol{r}'')\, \varrho(\boldsymbol{r}'',\tilde{\boldsymbol{r}}'') \\ &- \int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'') \lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''} \tau(\boldsymbol{r}'')\, \varrho(\tilde{\boldsymbol{r}}'',\boldsymbol{r}'') \\ &+ \int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'') \\ &+ 3 \int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\; v(\boldsymbol{r}'-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_2'') \\ &\qquad\times \sum_{\sigma_1',\sigma_2'} \Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'; \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2') \\ &+ \int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\mathrm{d}^d r_3''\; v(\boldsymbol{r}'-\boldsymbol{r}_1'')v(\boldsymbol{r}'-\boldsymbol{r}_2'')v(\boldsymbol{r}-\boldsymbol{r}_3'') \\ &\qquad\times \sum_{\sigma_1',\sigma_2',\sigma_3'} \Gamma^{(3)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2', \boldsymbol{r}_3''\sigma_3''; \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2', \boldsymbol{r}_3''\sigma_3'') \Big] \\ &\qquad\qquad\times \delta(\boldsymbol{r}-\boldsymbol{r}') \\ - \Big[& h_0(\boldsymbol{r})h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}')h_0(\boldsymbol{r}') + h_0(\boldsymbol{r}')h_0(\boldsymbol{r}) \\ &+ \big\{h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}')\big\} v(\boldsymbol{r}-\boldsymbol{r}') \\ &+ v(\boldsymbol{r}-\boldsymbol{r}')\big\{h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}')\big\} \\ &+ v(\boldsymbol{r}-\boldsymbol{r}')v(\boldsymbol{r}-\boldsymbol{r}') \Big] v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \\ &+ v(\boldsymbol{r}-\boldsymbol{r}')h_0(\boldsymbol{r})h_0(\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \\ &+ \Big[h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}') + 2v(\boldsymbol{r}-\boldsymbol{r}')\Big] v(\boldsymbol{r}-\boldsymbol{r}') \\ &\qquad\times \big\{\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}') + \mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big\} \\ &- v(\boldsymbol{r}-\boldsymbol{r}')\big\{\tau(\boldsymbol{r})\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}') + \tau(\boldsymbol{r}')\mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big\} \\ &+ v(\boldsymbol{r}-\boldsymbol{r}')v(\boldsymbol{r}-\boldsymbol{r}')\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}') - v(\boldsymbol{r}-\boldsymbol{r}')\mathcal{F}_\sigma(\boldsymbol{r},\boldsymbol{r}') \\ &- \int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')\tau(\boldsymbol{r}')v(\boldsymbol{r}-\boldsymbol{r}') \\ &\qquad\times \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}'\sigma, \boldsymbol{r}''\sigma'; \boldsymbol{r}\sigma, \boldsymbol{r}''\sigma') \\ &- \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\tau(\boldsymbol{r})v(\boldsymbol{r}-\boldsymbol{r}') \\ &\qquad\times \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}\sigma, \boldsymbol{r}''\sigma'; \boldsymbol{r}'\sigma, \boldsymbol{r}''\sigma') \\ &+ \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'') \lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''} \tau(\boldsymbol{r}'') \\ &\qquad\times \Big\{ \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}'\sigma, \tilde{\boldsymbol{r}}''\sigma'; \boldsymbol{r}\sigma, \boldsymbol{r}''\sigma') + \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}'\sigma, \boldsymbol{r}''\sigma'; \boldsymbol{r}\sigma, \tilde{\boldsymbol{r}}''\sigma') \Big\} \\ &- 2v(\boldsymbol{r}-\boldsymbol{r}') \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'') \\ &\qquad\times \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}'\sigma, \boldsymbol{r}''\sigma'; \boldsymbol{r}\sigma, \boldsymbol{r}''\sigma') \\ &- \int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'') \lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''} \tau(\boldsymbol{r}'')\, v(\boldsymbol{r}-\boldsymbol{r}'') \\ &\qquad\times \Big\{ \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}'\sigma, \boldsymbol{r}''\sigma'; \boldsymbol{r}\sigma, \tilde{\boldsymbol{r}}''\sigma') + \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}'\sigma, \tilde{\boldsymbol{r}}''\sigma'; \boldsymbol{r}\sigma, \boldsymbol{r}''\sigma') \Big\} \end{aligned}$$

$$+\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}')$$
$$-2v(\boldsymbol{r}-\boldsymbol{r}')\int \mathrm{d}^d r_1'' \mathrm{d}^d r_2''\; v(\boldsymbol{r}'-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_2'')$$
$$\times \sum_{\sigma_1',\sigma_2'} \Gamma^{(3)}(\boldsymbol{r}'\sigma,\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2';\boldsymbol{r}\sigma,\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2')\Big\}. \quad (194)$$

For the symmetric functions $\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and $\mathcal{F}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ see Appendix E. In Eq. (194) we have arranged the terms in such a way that the expected symmetry of $G_{\sigma;\infty_4}(\boldsymbol{r},\boldsymbol{r}')$ with respect to the exchange $\boldsymbol{r} \rightleftharpoons \boldsymbol{r}'$ (see Eq. (178) above; see also Appendix B) is made maximally explicit. In Appendix E we demonstrate the implicit symmetry of the contributions in Eq. (194) that are *not* manifestly symmetric with respect to $\boldsymbol{r} \rightleftharpoons \boldsymbol{r}'$. In Appendix D we prove that the explicitly asymmetric function $\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ on the RHS of Eq. (194) (for the defining expression see Eq. (D1)) is *identically* vanishing due to the assumed time-reversal symmetry of the GS. We have retained $\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (194) in order to preserve the most complete expression for $G_{\sigma;\infty_4}(\boldsymbol{r},\boldsymbol{r}')$ as deduced through carrying out a series of unbiased algebraic manipulations. Finally, from Eq. (194) one readily obtains $G_{0;\sigma;\infty_4}(\boldsymbol{r},\boldsymbol{r}') = \hbar\, h_{0;\sigma}(\boldsymbol{r})h_{0;\sigma}(\boldsymbol{r})h_{0;\sigma}(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}')$ (*cf.* Eqs. (171) and (182)).

1. Evaluation of $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$

Making use of the expression in Eq. (83) and employing the results in Eqs. (162) and (179), we straightforwardly obtain

$$\langle\boldsymbol{r}|G_{\sigma;\infty_2}G_{\sigma;\infty_3}|\boldsymbol{r}'\rangle = \hbar^2\Big\{\big[h_0(\boldsymbol{r})+v_H(\boldsymbol{r};[n])\big]$$
$$\times\big[h_0(\boldsymbol{r})h_0(\boldsymbol{r}')+h_0(\boldsymbol{r})v_H(\boldsymbol{r}';[n])+h_0(\boldsymbol{r}')v_H(\boldsymbol{r};[n])$$
$$+\mathcal{A}(\boldsymbol{r},\boldsymbol{r})+\int \mathrm{d}^d r''\; v^2(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')\big]\,\delta(\boldsymbol{r}-\boldsymbol{r}')$$
$$+\big[h_0(\boldsymbol{r})+v_H(\boldsymbol{r};[n])\big]$$
$$\times\big[-\big\{h_0(\boldsymbol{r})+h_0(\boldsymbol{r}')\big\}v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$$
$$-v^2(\boldsymbol{r}-\boldsymbol{r}')\,\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$$
$$+v(\boldsymbol{r}-\boldsymbol{r}')\big\{\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')+\mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big\}\big]$$
$$-\big[h_0(\boldsymbol{r}')h_0(\boldsymbol{r}')+v_H(\boldsymbol{r}';[n])h_0(\boldsymbol{r}')$$
$$+h_0(\boldsymbol{r}')v_H(\boldsymbol{r}';[n])+\mathcal{A}(\boldsymbol{r}',\boldsymbol{r}')$$
$$+\int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')n(\boldsymbol{r}'')v(\boldsymbol{r}''-\boldsymbol{r})\big]$$
$$\times v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$$
$$+\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r})$$
$$\times\big[\big\{h_0(\boldsymbol{r}'')+h_0(\boldsymbol{r}')\big\}v(\boldsymbol{r}''-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}'')$$
$$+v(\boldsymbol{r}''-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')$$
$$-v(\boldsymbol{r}''-\boldsymbol{r}')\big\{\mathcal{B}_\sigma(\boldsymbol{r}'',\boldsymbol{r}')+\mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r}'')\big\}\big]\Big\}, \quad (195)$$

from which we readily deduce that (see text preceding Eq. (171) above)

$$\langle\boldsymbol{r}|G_{0;\sigma;\infty_2}G_{0;\sigma;\infty_3}|\boldsymbol{r}'\rangle = \hbar^2 h_{0;\sigma}(\boldsymbol{r})h_{0;\sigma}(\boldsymbol{r})h_{0;\sigma}(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}'). \quad (196)$$

Further, in a similar manner to the above, we obtain

$$\langle\boldsymbol{r}|G_{\sigma;\infty_3}G_{\sigma;\infty_2}|\boldsymbol{r}'\rangle = \hbar^2\Big\{\big[h_0(\boldsymbol{r})h_0(\boldsymbol{r})$$
$$+h_0(\boldsymbol{r})v_H(\boldsymbol{r};[n])+v_H(\boldsymbol{r};[n])h_0(\boldsymbol{r})$$
$$+\mathcal{A}(\boldsymbol{r},\boldsymbol{r})+\int \mathrm{d}^d r''\; v^2(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')\big]$$
$$\times\Big(\big[h_0(\boldsymbol{r})+v_H(\boldsymbol{r};[n])\big]\,\delta(\boldsymbol{r}-\boldsymbol{r}')-v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\Big)$$
$$-\big[h_0(\boldsymbol{r}')+v_H(\boldsymbol{r}';[n])\big]\big[h_0(\boldsymbol{r})+h_0(\boldsymbol{r}')\big]v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$$
$$+\big[h_0(\boldsymbol{r}')+v_H(\boldsymbol{r}';[n])\big]v(\boldsymbol{r}-\boldsymbol{r}')$$
$$\times\big[\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')+\mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})-v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\big]$$
$$+\int \mathrm{d}^d r''\;\Big(\big[h_0(\boldsymbol{r})+h_0(\boldsymbol{r}'')+v(\boldsymbol{r}-\boldsymbol{r}'')\big]\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r})$$
$$-\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}'')-\mathcal{B}_\sigma(\boldsymbol{r}'',\boldsymbol{r})\Big)v(\boldsymbol{r}-\boldsymbol{r}'')$$
$$\times v(\boldsymbol{r}'-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}'')\Big\}, \quad (197)$$

from which we infer that

$$\langle\boldsymbol{r}|G_{0;\sigma;\infty_3}G_{0;\sigma;\infty_2}|\boldsymbol{r}'\rangle = \hbar^2 h_{0;\sigma}(\boldsymbol{r})h_{0;\sigma}(\boldsymbol{r})h_{0;\sigma}(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}'). \quad (198)$$

Combining the above results in accordance with the expression in Eq. (75) (or Eq. (78)), we finally arrive at (below $\varrho \equiv \sum_{\sigma'}\varrho_{\sigma'}$ and $n \equiv \sum_{\sigma'} n_{\sigma'}$)

$$\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{\hbar}\Big\{\Big[v_H^3(\boldsymbol{r};[n])$$
$$-v_H(\boldsymbol{r};[n])v_H(\boldsymbol{r}';[n])h_0(\boldsymbol{r})-2v_H(\boldsymbol{r};[n])\mathcal{A}(\boldsymbol{r},\boldsymbol{r})$$
$$-2v_H(\boldsymbol{r};[n])\int \mathrm{d}^d r''\; v^2(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')$$
$$+\mathcal{A}(\boldsymbol{r},\boldsymbol{r}')h_0(\boldsymbol{r})$$
$$+\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')n(\boldsymbol{r}'')h_0(\boldsymbol{r}')$$
$$+\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''}\tau(\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'')\varrho(\boldsymbol{r}'',\tilde{\boldsymbol{r}}'')$$
$$-\int \mathrm{d}^d r''\; v^2(\boldsymbol{r}-\boldsymbol{r}'')\lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''}\tau(\boldsymbol{r}'')\varrho(\tilde{\boldsymbol{r}}'',\boldsymbol{r}'')$$
$$+\int \mathrm{d}^d r''\; v^3(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')$$
$$+3\int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\; v^2(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_2'')$$
$$\times\sum_{\sigma_1',\sigma_2'}\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2';\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2')$$
$$+\int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\mathrm{d}^d r_3''\; v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_2'')v(\boldsymbol{r}-\boldsymbol{r}_3'')$$

$$
\begin{aligned}
&\times \sum_{\sigma_1',\sigma_2',\sigma_3'} \Gamma^{(3)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2', \boldsymbol{r}_3''\sigma_3'; \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2', \boldsymbol{r}_3''\sigma_3')\Big] \\
&\qquad\qquad\qquad\qquad \times\delta(\boldsymbol{r}-\boldsymbol{r}') \\
&-\Big[v_H^2(\boldsymbol{r};[n]) + v_H^2(\boldsymbol{r}';[n]) + v_H(\boldsymbol{r};[n])v_H(\boldsymbol{r}';[n]) \\
&\quad -v_H(\boldsymbol{r};[n])v(\boldsymbol{r}-\boldsymbol{r}') - v_H(\boldsymbol{r}';[n])v(\boldsymbol{r}-\boldsymbol{r}') \\
&\quad -v_H(\boldsymbol{r};[n])h_0(\boldsymbol{r}) - v_H(\boldsymbol{r}';[n])h_0(\boldsymbol{r}') \\
&\quad -\mathcal{A}(\boldsymbol{r},\boldsymbol{r}) - \mathcal{A}(\boldsymbol{r}',\boldsymbol{r}') \\
&\quad -\int \mathrm{d}^d r''\; \{v^2(\boldsymbol{r}-\boldsymbol{r}'') + v^2(\boldsymbol{r}'-\boldsymbol{r}'')\}\, n(\boldsymbol{r}'') \\
&\quad +v(\boldsymbol{r}-\boldsymbol{r}')\big\{h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}')\big\} + v^2(\boldsymbol{r}-\boldsymbol{r}')\Big] \\
&\qquad\qquad\qquad \times v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \\
&+\frac{1}{2}v^2(\boldsymbol{r}-\boldsymbol{r}')\big\{h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}')\big\}\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \\
&+\big\{v_H(\boldsymbol{r};[n]) + v_H(\boldsymbol{r}';[n])\big\} \\
&\quad \times\Big\{ \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r}') \\
&\qquad -v(\boldsymbol{r}-\boldsymbol{r}')\big[\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}') + \mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big]\Big\} \\
&+\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')v_H(\boldsymbol{r}'';[n]) \\
&\qquad\qquad\qquad \times\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r}') \\
&-\int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}'-\boldsymbol{r}_2'')v(\boldsymbol{r}_1''-\boldsymbol{r}_2'') \\
&\qquad\qquad \times\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}_1'')\varrho_\sigma(\boldsymbol{r}_1'',\boldsymbol{r}_2'')\varrho_\sigma(\boldsymbol{r}_2'',\boldsymbol{r}') \\
&-\int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r}')h_0(\boldsymbol{r}'') \\
&\qquad\qquad\qquad \times v(\boldsymbol{r}''-\boldsymbol{r})\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}'') \\
&-\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v^2(\boldsymbol{r}'-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}'')\,\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r}') \\
&-\int \mathrm{d}^d r''\; v^2(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}'')\,\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r}) \\
&+\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r}) \\
&\qquad\qquad \times\big\{\mathcal{B}_\sigma(\boldsymbol{r}'',\boldsymbol{r}') + \mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r}'')\big\} \\
&+\int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r}') \\
&\qquad\qquad \times\big\{\mathcal{B}_\sigma(\boldsymbol{r}'',\boldsymbol{r}) + \mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}'')\big\} \\
&+\frac{3}{2}v^2(\boldsymbol{r}-\boldsymbol{r}')\big\{\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}') + \mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big\} \\
&-\frac{1}{2}v(\boldsymbol{r}-\boldsymbol{r}')\big\{\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}') + \mathcal{G}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big\} \\
&+\frac{1}{2}v(\boldsymbol{r}-\boldsymbol{r}')\big\{h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}')\big\}\big\{\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}') + \mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big\} \\
&-v(\boldsymbol{r}-\boldsymbol{r}')\big\{\tau(\boldsymbol{r})\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}') + \tau(\boldsymbol{r}')\mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big\} \\
&-\int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')\tau(\boldsymbol{r}')v(\boldsymbol{r}-\boldsymbol{r}') \\
&\qquad\qquad \times\sum_{\sigma'}\Gamma^{(2)}(\boldsymbol{r}'\sigma, \boldsymbol{r}''\sigma'; \boldsymbol{r}\sigma, \boldsymbol{r}''\sigma') \\
&-\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\tau(\boldsymbol{r})v(\boldsymbol{r}-\boldsymbol{r}') \\
&\qquad\qquad \times\sum_{\sigma'}\Gamma^{(2)}(\boldsymbol{r}\sigma, \boldsymbol{r}''\sigma'; \boldsymbol{r}'\sigma, \boldsymbol{r}''\sigma') \\
&-2v(\boldsymbol{r}-\boldsymbol{r}')\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'') \\
&\qquad\qquad \times\sum_{\sigma'}\Gamma^{(2)}(\boldsymbol{r}'\sigma, \boldsymbol{r}''\sigma'; \boldsymbol{r}\sigma, \boldsymbol{r}''\sigma') \\
&+\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''}\tau(\boldsymbol{r}'') \\
&\qquad\qquad \times\Big\{\sum_{\sigma'}\Gamma^{(2)}(\boldsymbol{r}'\sigma, \tilde{\boldsymbol{r}}''\sigma'; \boldsymbol{r}\sigma, \boldsymbol{r}''\sigma') \\
&\qquad\qquad\quad +\sum_{\sigma'}\Gamma^{(2)}(\boldsymbol{r}'\sigma, \boldsymbol{r}''\sigma'; \boldsymbol{r}\sigma, \tilde{\boldsymbol{r}}''\sigma')\Big\} \\
&-\int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')\lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''}\tau(\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'') \\
&\qquad\qquad \times\Big\{\sum_{\sigma'}\Gamma^{(2)}(\boldsymbol{r}'\sigma, \tilde{\boldsymbol{r}}''\sigma'; \boldsymbol{r}\sigma, \boldsymbol{r}''\sigma') \\
&\qquad\qquad\quad +\sum_{\sigma'}\Gamma^{(2)}(\boldsymbol{r}'\sigma, \boldsymbol{r}''\sigma'; \boldsymbol{r}\sigma, \tilde{\boldsymbol{r}}''\sigma')\Big\} \\
&+\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}') \\
&-2v(\boldsymbol{r}-\boldsymbol{r}')\int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}'-\boldsymbol{r}_2'') \\
&\quad \times\sum_{\sigma_1',\sigma_2'}\Gamma^{(3)}(\boldsymbol{r}'\sigma, \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'; \boldsymbol{r}\sigma, \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2')\Big\}. \qquad (199)
\end{aligned}
$$

For the *asymmetric* function $\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ see Eq. (E18). It is readily verified that the above expression appropriately satisfies the required symmetry property (see Appendix B) $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') \equiv \Sigma_{\sigma;\infty_2}(\boldsymbol{r}',\boldsymbol{r})$. As in the case of $G_{\sigma;\infty_4}(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (194), we have retained the *identically* vanishing function $\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ (see Appendix D; see also text following Eq. (194)) in the above expression for $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ so as to preserve the most complete expression for this function as obtained through performing a sequence of unbiased calculations.

2. The case of Coulomb-interacting fermions in the thermodynamic limit

Here we consider the case in which $v \equiv v_c$ and $d = 3$. Similar to $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')$ and $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$, whose expressions as presented in Eqs. (173) and (185) respectively involve integrals that owing to the long range of v_c are unbounded for $v \equiv v_c$, $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ as expressed in Eq. (199) is determined in terms of integrals that owing to the latter property of v_c are unbounded when v herein is identified with v_c (and d with 3). Consequently, the expression in Eq. (199) must be reformulated prior to effecting the substitution $v \rightharpoonup v_c$ (see § II.B). A second aspect associated with $v_c(\boldsymbol{r}-\boldsymbol{r}')$ that gains prominence in the expression for $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ and remains prominent in the expressions for $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, for *all* $m>2$, is its divergence like $1/\|\boldsymbol{r}-\boldsymbol{r}'\|$ for $\|\boldsymbol{r}-\boldsymbol{r}'\|\to 0$ (see however footnote 27). [89]

A systematic analysis of the expression on the RHS of Eq. (199) reveals that (for some details see Appendices F and G) $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ is fundamentally *unbounded*, that is in contrast with $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')$ and $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ the unbounded contributions to the constituent terms of $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ do *not* fully cancel. As the SE $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ is itself a bounded function almost everywhere (see footnote 54), it follows that these contributions to $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ *must* have their compensating counterparts in the expressions for $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ corresponding to $m>2$ (*cf.* § II.B). A thorough inspection of the expression on the RHS of Eq. (199) further reveals that the *explicitly*-presented functions $h_0(\boldsymbol{r})$ and $v_H(\boldsymbol{r};[n])$ in this expression *cannot* be brought into such combinations as $h_0(\boldsymbol{r})+v_H(\boldsymbol{r};[n])$, $h_0(\boldsymbol{r})-h_0(\boldsymbol{r}')$ or $v_H(\boldsymbol{r};[n])-v_H(\boldsymbol{r}';[n])$ where the divergent contribution ϖ_κ, corresponding to $\kappa\downarrow 0$, is fully cancelled. [90] This observation implies that some unbounded contributions involving ϖ_κ must necessarily be *implicit* in the expression on the RHS of Eq. (199), which detailed considerations show indeed to be the case. These considerations have led us to the complete identification of the set of unbounded and non-integrable functions in the expression on the RHS of Eq. (199) (see criteria (A) - (C) in § II.B) together with their compensating counterparts (see § II.B) in the formal expressions for $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ with $m>2$.

Our analyses demonstrate that $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ contains *four* fundamentally *unbounded* contributions, of which three originate from the *local* part of $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ (that is that part which in Eq. (199) is post-multiplied by $\delta(\boldsymbol{r}-\boldsymbol{r}')$), and the fourth originates from what in the case of $v\not\equiv v_c$ is a (bounded) *non*-local contribution to $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$; as $v\rightharpoonup v_c$, this is shown to transform into a *local* unbounded contribution [91] (see text following Eq. (185) above). It follows that all unbounded contributions to $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$, arising from the identification of v with v_c and d with 3, are local. It is interesting to mention that the latter fourth contribution (i.e. $\mathcal{I}_4$ in Eq. (203) below) turns out to belong to the same category as one of the former three local unbounded contributions (i.e. $\mathcal{I}_3$ in Eq. (202) below) and its effect is one of rendering $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ *explicitly* dependent upon $\bar{\sigma}$, the totality of the spin components complementary to σ (see the definition in the text following Eq. (19) above; see also Eq. (209) below). More importantly, the regularized expression (see Appendix G) corresponding to these two contributions, that is $\mathcal{I}_3$ and $\mathcal{I}_4$, which is shown to be proportional to $\sum_{\sigma'\neq\sigma} n_{\sigma'}(\boldsymbol{r})-n_\sigma(\boldsymbol{r})\equiv n_{\bar{\sigma}}(\boldsymbol{r})-n_\sigma(\boldsymbol{r})$ (for the case of spin-1/2 fermions, this amounts to $n_\downarrow(\boldsymbol{r})-n_\uparrow(\boldsymbol{r})$ when $\sigma=\uparrow$), has a distinctive asymptotic behaviour for $|z|\to\infty$: it decays in magnitude like $1/|z|^{3/2}$, to be compared with the decay of other contributions to the large-$|z|$ AS for $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ following $\Sigma_{\sigma;\infty_1}/z$, which depend on $\ln(-z/\varepsilon_0)/z^2$, $1/z^2$, etc. (here ε_0 denotes an arbitrary constant energy). The dependence of the mentioned contribution on $n_{\bar{\sigma}}(\boldsymbol{r})-n_\sigma(\boldsymbol{r})$ provides a direct means by which to establish the existence and to determine the magnitude of this possible local imbalance in the distribution of the particles with spin σ with respect to that of the remaining particles. Aside from the interest of this result to the interpretation of the experimental *inverse* photo-emission data (see Eqs. (234) and (239) below), it unequivocally demonstrates that models that through neglect of Umklapp processes do not account for the possibility of *local* imbalance in the distribution of particles with different spins (to be distinguished from the long-range ordering of spins, corresponding to, e.g., ferromagnetism or anti-ferromagnetism) are *not* capable of manifesting the latter asymptotic behaviour at large valued of $|z|$. Further, since this particular behaviour owes its existence to the $1/\|\boldsymbol{r}-\boldsymbol{r}'\|$ singularity of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ at $\boldsymbol{r}=\boldsymbol{r}'$, it is equally not accounted for in theoretical considerations based on models that involve bounded interaction potentials, such as is the case in the Hubbard model (for example Montorsi (1992), Gebhard (1997)) involving a finite *intra*-atomic interaction potential.

For concreteness, we now present the aforementioned *four* fundamentally unbounded contributions in the expression on the RHS of Eq. (199) specific to $v\equiv v_c$ in $d=3$. An immediate and unequivocal recognition of these contributions in Eq. (199) is *not* possible, since a substantial reorganization of terms in Eq. (199) will have to be effected before the following contributions are deduced (see Appendices F and G for some details). We have

$$\mathcal{I}_1 := \int \mathrm{d}^d r''\; v^3(\boldsymbol{r}-\boldsymbol{r}'')\, n(\boldsymbol{r}'')\, \delta(\boldsymbol{r}-\boldsymbol{r}'); \tag{200}$$

$$\mathcal{I}_2 := \int \mathrm{d}^d r_1'' \mathrm{d}^d r_2''\; v^2(\boldsymbol{r}-\boldsymbol{r}_1'') v(\boldsymbol{r}-\boldsymbol{r}_2'')$$

[89] We point out that $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ stands on the 'boundary' where the behaviours of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ at both small and large $\|\boldsymbol{r}-\boldsymbol{r}'\|$ play equally significant roles; concerning $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, the behaviour of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ at large $\|\boldsymbol{r}-\boldsymbol{r}'\|$ is dominant for $m=0,1$, while this dominance is shared by the behaviour of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ at small $\|\boldsymbol{r}-\boldsymbol{r}'\|$ for $m\geq 2$.

[90] Here, as in other places in the present work, $v_H(\boldsymbol{r};[n])$ is defined according to Eq. (14) with v' as defined in Eq. (13); neglect in Eq. (13) of the cut-off function $\exp(-\kappa\|\boldsymbol{r}-\boldsymbol{r}'\|)$, with $\kappa\downarrow 0$, can lead to *ambiguity* in the expressions, even at the formal level where the possible boundedness of certain integrals is *not* at issue.

[91] By 'local unbounded' contribution we refer to a two-point function of the form $f(\boldsymbol{r},\boldsymbol{r}')\,\delta(\boldsymbol{r}-\boldsymbol{r}')$, with $f(\boldsymbol{r},\boldsymbol{r}')$ an unbounded function for $\|\boldsymbol{r}-\boldsymbol{r}'\|\to 0$.

$$\times \sum_{\sigma_1',\sigma_2'} \Big[\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'; \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2') - n_{\sigma_1'}(\boldsymbol{r}_1'')n_{\sigma_2'}(\boldsymbol{r}_2'')\Big] \times\delta(\boldsymbol{r}-\boldsymbol{r}'); \quad (201)$$

$$\mathcal{I}_3 := \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')\big(\tau(\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'')\big)\,\delta(\boldsymbol{r}-\boldsymbol{r}'); \quad (202)$$

$$\mathcal{I}_4 := -2v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\big(\tau(\boldsymbol{r})v(\boldsymbol{r}-\boldsymbol{r}')\big). \quad (203)$$

It can be easily verified that for $v \equiv v_c$ in $d=3$, $\mathcal{I}_1$ is unbounded for two reasons: firstly, the singularity of $v_c^3(\boldsymbol{r}-\boldsymbol{r}'')$ at $\boldsymbol{r}''=\boldsymbol{r}$ is *not* integrable, and secondly, excluding a finite neighbourhood of $\boldsymbol{r}''=\boldsymbol{r}$, $\mathcal{I}_1$ further diverges as the volume of the system, Ω, tends to infinity.[92] It can also be shown (see Appendix F) that similarly $\mathcal{I}_2$ diverges as $\Omega\to\infty$. However, since the leading term in the large-$\|\boldsymbol{r}_1''\|$ AS of the integral over $\boldsymbol{r}_2''$ in Eq. (201) is equal to $-v_c(\boldsymbol{r}-\boldsymbol{r}_1'')n(\boldsymbol{r}_1'')$ (see Eq. (F140) and footnote 135), the sum (see Eq. (F133))

$$\mathcal{I}_1+\mathcal{I}_2 =: \mathcal{M}(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}') \quad (204)$$

does *not* suffer from the latter problem of diverging in consequence of $\Omega\to\infty$; the integrand corresponding to $\mathcal{M}(\boldsymbol{r})$, as originating from $\mathcal{I}_1$, is non-integrable, however, owing to the indicated singularity of $v_c^3(\boldsymbol{r}-\boldsymbol{r}'')$ at $\boldsymbol{r}''=\boldsymbol{r}$. This can be remedied through a summation over an infinite number of non-integrable counterparts pertaining to $\{\Sigma_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')\,\|\, p>2\}$; we present the details of this renormalization procedure in Appendix F.

Following Eq. (16), we have (see Eq. (3))

$$\tau(\boldsymbol{r})v_c(\boldsymbol{r}-\boldsymbol{r}') = \frac{\hbar^2 e^2}{2m_e\epsilon_0}\,\delta(\boldsymbol{r}-\boldsymbol{r}'), \quad (205)$$

which upon substitution into the expressions on the RHSs of Eqs. (202) and (203), with $v\equiv v_c$, results in

$$\mathcal{I}_3 \rightharpoonup \frac{\hbar^2 e^2}{2m_e\epsilon_0} v_c(\boldsymbol{r}-\boldsymbol{r}')n(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}'), \quad (206)$$

$$\mathcal{I}_4 \rightharpoonup -\frac{\hbar^2 e^2}{m_e\epsilon_0} v_c(\boldsymbol{r}-\boldsymbol{r}')n_\sigma(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}'), \quad (207)$$

both of which are unbounded as a consequence of the combination of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ with $\delta(\boldsymbol{r}-\boldsymbol{r}')$ (see footnote 91 and the text citing it). In Appendix G we consider the regularization of $\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})$ in

$$\mathcal{I}_3+\mathcal{I}_4 =: \mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}'), \quad (208)$$

where

$$\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r}) := \int \mathrm{d}^3 r''\; v_c(\boldsymbol{r}-\boldsymbol{r}'')\big[n_{\bar\sigma}(\boldsymbol{r}'')-n_\sigma(\boldsymbol{r}'')\big] \times\big(\tau(\boldsymbol{r}'')v_c(\boldsymbol{r}-\boldsymbol{r}'')\big). \quad (209)$$

Following the above considerations, we now present the expression for $\widetilde{\Sigma}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'|z)$ (see Eq. (110) above) pertaining to a macroscopic system for which we use the decomposition of $n(\boldsymbol{r})$ as presented in Eq. (12). In the expressions that we provide below, the contribution of $v_H(\boldsymbol{r};[n_0])$, which may or may not be unbounded (as nowhere do we require identity of v with v_c), is *naturally* cancelled against a counterpart in $h_0(\boldsymbol{r})$ (see Eq. (43) above); with reference to Eqs. (15) and (172), we should bear mind that the explicit expression for ϖ_κ in Eq. (5) is specific to Coulomb interacting fermion systems in $d=3$. The expression for $\widetilde{\Sigma}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'|z)$ that we present below is therefore specifically, but *not* exclusively, suitable for the cases corresponding to $v\equiv v_c$ in $d=3$.

With reference to Eq. (110) (see the considerations in § III.E.2), we write

$$\widetilde{\Sigma}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'|z) \equiv \Sigma^{\mathrm{r}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') + \Sigma^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') + \widetilde{\Sigma}^{\mathrm{s}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'\|z), \quad (210)$$

where (see Eq. (199) above; below we suppress the identically vanishing function $\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ that is encountered in Eq. (199); see Appendix D)

$$\begin{aligned}
\Sigma^{\mathrm{r}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{\hbar}\Big\{ &\Big(\mathcal{A}'(\boldsymbol{r},\boldsymbol{r}')\big(\tau(\boldsymbol{r})+u(\boldsymbol{r})+v_H(\boldsymbol{r};[n'])\big)\\
&-\frac{\hbar^2}{2m_e}\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')[\boldsymbol{\nabla}_{\boldsymbol{r}''}v(\boldsymbol{r}-\boldsymbol{r}'')]\cdot[\boldsymbol{\nabla}_{\boldsymbol{r}''}n(\boldsymbol{r}'')]\\
&+\mathcal{L}''(\boldsymbol{r})\Big)\,\delta(\boldsymbol{r}-\boldsymbol{r}')\\
&+\big(\mathcal{B}''_\sigma(\boldsymbol{r},\boldsymbol{r}')+\mathcal{B}''_\sigma(\boldsymbol{r}',\boldsymbol{r})\big)\big(\tau(\boldsymbol{r})v(\boldsymbol{r}-\boldsymbol{r}')\big)\\
&+\big(\mathcal{A}'(\boldsymbol{r},\boldsymbol{r})+\mathcal{A}'(\boldsymbol{r}',\boldsymbol{r}')\big)v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\\
&+\frac{1}{2}v(\boldsymbol{r}-\boldsymbol{r}')\big(v_H(\boldsymbol{r};[n'])-v_H(\boldsymbol{r}';[n'])\big)\\
&\quad\times\big(\tau(\boldsymbol{r})-\tau(\boldsymbol{r}')+u(\boldsymbol{r})-u(\boldsymbol{r}')\\
&\quad+v_H(\boldsymbol{r};[n'])-v_H(\boldsymbol{r}';[n'])\big)\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\\
&+\frac{1}{2}v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\big(\tau(\boldsymbol{r})v_H(\boldsymbol{r};[n'])+\tau(\boldsymbol{r}')v_H(\boldsymbol{r}';[n'])\big)\\
&-\frac{1}{2}v^2(\boldsymbol{r}-\boldsymbol{r}')\big(\tau(\boldsymbol{r})+\tau(\boldsymbol{r}')+u(\boldsymbol{r})+u(\boldsymbol{r}')\\
&\quad+v_H(\boldsymbol{r};[n'])+v_H(\boldsymbol{r}';[n'])\big)\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\\
&+\frac{1}{2}v(\boldsymbol{r}-\boldsymbol{r}')\big(\tau(\boldsymbol{r})+\tau(\boldsymbol{r}')+u(\boldsymbol{r})+u(\boldsymbol{r}')\\
&\quad+v(\boldsymbol{r}-\boldsymbol{r}')\big)\big(\mathcal{B}''_\sigma(\boldsymbol{r},\boldsymbol{r}')+\mathcal{B}''_\sigma(\boldsymbol{r}',\boldsymbol{r})\big)\\
&+v(\boldsymbol{r}-\boldsymbol{r}')\big(v_H(\boldsymbol{r};[n'])\mathcal{B}''_\sigma(\boldsymbol{r}',\boldsymbol{r})+v_H(\boldsymbol{r}';[n'])\mathcal{B}''_\sigma(\boldsymbol{r},\boldsymbol{r}')\big)\\
&-\frac{1}{2}v(\boldsymbol{r}-\boldsymbol{r}')\big(\mathcal{G}''_\sigma(\boldsymbol{r},\boldsymbol{r}')+\mathcal{G}''_\sigma(\boldsymbol{r}',\boldsymbol{r})\big)\\
&-2v(\boldsymbol{r}-\boldsymbol{r}')\mathcal{K}'''_\sigma(\boldsymbol{r},\boldsymbol{r}')\\
&+\frac{\hbar^2}{m_e}v(\boldsymbol{r}-\boldsymbol{r}')\big([\boldsymbol{\nabla}_{\boldsymbol{r}}v(\boldsymbol{r}-\boldsymbol{r}')]\cdot[\boldsymbol{\nabla}_{\boldsymbol{r}}\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})]
\end{aligned}$$

[92] To be precise, by employing the v' corresponding to v_c in Eq. (13), the calculated $\mathcal{I}_1$ diverges (logarithmically) as $\kappa\downarrow 0$.

$$
+[\nabla_{\boldsymbol{r}'} v(\boldsymbol{r}-\boldsymbol{r}')]\cdot[\nabla_{\boldsymbol{r}'}\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})]\big)
-\frac{\hbar^2}{2m_e} v(\boldsymbol{r}-\boldsymbol{r}')\big([\nabla_{\boldsymbol{r}} v_H(\boldsymbol{r};[n'])]\cdot[\nabla_{\boldsymbol{r}}\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})]
+[\nabla_{\boldsymbol{r}'} v_H(\boldsymbol{r}';[n'])]\cdot[\nabla_{\boldsymbol{r}'}\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})]\big)
+v(\boldsymbol{r}-\boldsymbol{r}')\int \mathrm{d}^d r''\sum_{\sigma'}\big(\Gamma^{(2)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma')
-n_{\sigma'}(\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\big)
\times\big(\tau(\boldsymbol{r})v(\boldsymbol{r}-\boldsymbol{r}'')+\tau(\boldsymbol{r}')v(\boldsymbol{r}'-\boldsymbol{r}'')\big)
-\frac{\hbar^2}{m_e}\int \mathrm{d}^d r''\,\big(v(\boldsymbol{r}-\boldsymbol{r}')[\nabla_{\boldsymbol{r}} v(\boldsymbol{r}-\boldsymbol{r}'')]
-v(\boldsymbol{r}-\boldsymbol{r}'')[\nabla_{\boldsymbol{r}} v(\boldsymbol{r}-\boldsymbol{r}')]\big)
\cdot\big[\nabla_{\boldsymbol{r}}\sum_{\sigma'}\big(\Gamma^{(2)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma')-n_{\sigma'}(\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\big)\big]
-\frac{\hbar^2}{m_e}\int \mathrm{d}^d r''\,\big(v(\boldsymbol{r}-\boldsymbol{r}')[\nabla_{\boldsymbol{r}'} v(\boldsymbol{r}'-\boldsymbol{r}'')]
-v(\boldsymbol{r}'-\boldsymbol{r}'')[\nabla_{\boldsymbol{r}'} v(\boldsymbol{r}-\boldsymbol{r}')]\big)
\cdot\big[\nabla_{\boldsymbol{r}'}\sum_{\sigma'}\big(\Gamma^{(2)}(\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}'\sigma,\boldsymbol{r}''\sigma')-n_{\sigma'}(\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\big)\big]
-\frac{\hbar^2}{m_e}\int \mathrm{d}^d r''\,[\nabla_{\boldsymbol{r}''} v(\boldsymbol{r}-\boldsymbol{r}'')]\cdot[\nabla_{\boldsymbol{r}''} v(\boldsymbol{r}'-\boldsymbol{r}'')]
\times\sum_{\sigma'}\Gamma^{(2)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma')
-\frac{\hbar^2}{2m_e}\int \mathrm{d}^d r''\,[\nabla_{\boldsymbol{r}''} v(\boldsymbol{r}-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}'')]
\cdot[\nabla_{\boldsymbol{r}''} v(\boldsymbol{r}'-\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}'')]
-\int \mathrm{d}^d r''\, v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')
\times\big(u(\boldsymbol{r}'')+v_H(\boldsymbol{r}'';[n'])-v(\boldsymbol{r}-\boldsymbol{r}'')-v(\boldsymbol{r}'-\boldsymbol{r}'')\big)
\times\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}'',\boldsymbol{r})
-\int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\, v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}'-\boldsymbol{r}_2'')v(\boldsymbol{r}_1''-\boldsymbol{r}_2'')
\times\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}_1'')\varrho_\sigma(\boldsymbol{r}_1'',\boldsymbol{r}_2'')\varrho_\sigma(\boldsymbol{r}_2'',\boldsymbol{r}')\Big\}, \quad (211)
$$

$$
\Sigma^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') = -\frac{1}{\hbar}\, v^3(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}), \quad (212)
$$

$$
\widetilde{\Sigma}^{\mathrm{s}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'\|z) = \frac{1}{\hbar}\Big\{\mathsf{M}^{\mathrm{r}}_{\infty_2}(\boldsymbol{r})+\widetilde{\mathsf{M}}^{\mathrm{s}}_{\infty_2}(\boldsymbol{r}\|z)
+\widetilde{\mathsf{T}}^{\mathrm{s}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}\|z)\Big\}\,\delta(\boldsymbol{r}-\boldsymbol{r}'). \quad (213)
$$

For functions $\mathcal{A}'$, $\mathcal{B}''_\sigma$, $\mathcal{G}''_\sigma$ and $\mathcal{K}'''_\sigma$, their definitions and significant properties, see Appendix F (see specifically Eqs. (F3), (F113), (F119) and (F127) respectively). For the explicit expressions for $\mathsf{M}^{\mathrm{r}}_{\infty_2}(\boldsymbol{r})$, $\widetilde{\mathsf{M}}^{\mathrm{s}}_{\infty_2}(\boldsymbol{r}\|z)$ and $\widetilde{\mathsf{T}}^{\mathrm{s}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}\|z)$ see Eqs. (F159), (F160) and (G15) respectively. The 'singular' contribution arising from $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ that initializes the infinite series (i.e. that underlying the required regularization process) of unbounded terms whose relevant asymptotic contribution to $\widetilde{\Sigma}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'|z)$ for $|z|\to\infty$ is $\widetilde{\Sigma}^{\mathrm{s}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'\|z)$ on the RHS of Eq. (213), is the following (see Eqs. (204) and (208) above)

$$
\Sigma^{\mathrm{s}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') \equiv \frac{1}{\hbar}\big\{\mathcal{M}(\boldsymbol{r})+\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})\big\}\,\delta(\boldsymbol{r}-\boldsymbol{r}'), \quad (214)
$$

where $\mathcal{M}(\boldsymbol{r})$ is defined in Eq. (F133) below and $\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})$ in Eq. (209) above (see Appendix G). We note that $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')\equiv\Sigma^{\mathrm{r}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')+\Sigma^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')+\Sigma^{\mathrm{s}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$, with the constituent parts being those presented in Eqs. (211), (212) and (214) respectively, *is* fully identical with $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (199). This follows from the fact that *no* specific aspect of v_c has been assumed in arriving at the expressions in Eqs. (211), (212) and (214). In contrast, the expression for $\widetilde{\Sigma}^{\mathrm{s}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'\|z)$ in Eq. (213), to be contrasted with $\Sigma^{\mathrm{s}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (214), *is* specific to $v\equiv v_c$ in $d=3$ and has its origin in an infinite number of terms in the *formal* expressions pertaining to $\{\Sigma^{\mathrm{s}}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')\,\|\,p\geq 2\}$. We note that $\widetilde{\mathsf{T}}^{\mathrm{s}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}\|z)\equiv 0$ for $n_\sigma(\boldsymbol{r})\equiv n_{\bar{\sigma}}(\boldsymbol{r})$ (see Eq. (G15)).

While employing the expression in Eq. (211) for $v\equiv v_c$ in $d=3$, the following simplified results (see Eq. (205) above and footnote 26) are at one's disposal:

$$
\big(\mathcal{B}''_\sigma(\boldsymbol{r},\boldsymbol{r}')+\mathcal{B}''_\sigma(\boldsymbol{r}',\boldsymbol{r})\big)\tau(\boldsymbol{r})v_c(\boldsymbol{r}-\boldsymbol{r}')
= \frac{\hbar^2 e^2}{m_e\epsilon_0}\,\mathcal{B}''_\sigma(\boldsymbol{r},\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}') \quad (215)
$$

and

$$
\tau(\boldsymbol{r})v_H(\boldsymbol{r};[n'])+\tau(\boldsymbol{r}')v_H(\boldsymbol{r}';[n'])
= \frac{\hbar^2 e^2}{2m_e\epsilon_0}\,\big(n'(\boldsymbol{r})+n'(\boldsymbol{r}')\big). \quad (216)
$$

As can be easily verified from Eq. (F112) (see also Eq. (F113)), in contrast with $\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r})$, $\mathcal{B}''_\sigma(\boldsymbol{r},\boldsymbol{r})$ is *bounded* and well-defined. For the cases corresponding to $v\not\equiv v_c$, the LHS of Eq. (215) accounts for a *non*-local contribution to $\Sigma^{\mathrm{r}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ which, as the RHS shows, transforms into a *local* contribution to $\Sigma^{\mathrm{r}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ in the cases corresponding to $v\equiv v_c$. This aspect is significant in that it demonstrates that *any* local approximation to $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$, designed for an *arbitrary* two-body potential v, will fail correctly to reproduce the local part of $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ when applied to cases where $v\equiv v_c$ (and $d=3$). In this connection we recall that a crucial contribution to $\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})$, namely $\mathcal{I}_4$ in Eq. (203), and consequently $\widetilde{\mathsf{T}}^{\mathrm{s}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}\|z)$ (see Eq. (G15)), [93] has

[93] The first term (corresponding to $m=1$) in the series representation of $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$ in Eq. (G1), is simply $z^{-2}\,\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})$ where $\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})$ is introduced in Eq. (209).

its origin in what for a general v amounts to a *non*-local term in the expression for $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$. As we explicitly demonstrate in § IV, in the first-order perturbation series for $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ in terms of the dynamical screened interaction function $W(\varepsilon)$ (Hubbard 1957), as opposed to the static bare interaction function v (here, v_c), *non*-local terms are missing altogether in the corresponding expression for $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ (which we denote by $\Sigma^{(1)}_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$; see Eq. (257) below); further, the absence of a crucial non-local contribution (namely, $\mathcal{I}_4$ introduced in Eq. (203) above) in the first-order counterpart of $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$, that is $\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ (see Eq. (267) below), results in $\widetilde{\mathsf{T}}^{(1)}(\boldsymbol{r};z)$ (see Eq. (277) below), to be contrasted with $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$ (see Eq. (209) above) in the exact treatment.

For completeness, as can be seen from Eqs. (210), (213) and (G15), in general, in the cases corresponding to $v \equiv v_c$, $\hbar^{-1}\widetilde{\mathsf{T}}^{\rm s}_{\sigma,\bar{\sigma}}(\boldsymbol{r}\|z)\,\delta(\boldsymbol{r}-\boldsymbol{r}')$ is a dominant contribution to the local part of the *regularized* $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$, that is $\widetilde{\Sigma}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'|z)$; for increasing values of $|z|$, this contribution decays *most slowly* in comparison with *all* other asymptotic contributions to $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ that follow $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')/z$ (see Eq. (112) above). This again makes evident that *non*-local contributions to $\Sigma_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ can acquire considerable significance when $v \equiv v_c$.

We close this Section by pointing out the important fact that, *independent* of whether the GS of the system under consideration is metallic or insulating, $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ involves both unbounded and non-integrable contributions (see Eqs. (214) and (212) respectively) in cases where $v \equiv v_c$ in $d = 3$ (*not* exclusively, however). Since regularization of the unbounded contributions to $\Sigma^{\rm s}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (214) requires a summation over an *infinite* number of terms pertaining to $\Sigma_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$, $p > 2$, in view of the direct relationship between $\Sigma_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ and the many-body perturbation series for $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ in terms of the bare v and the *exact* G_{σ} (see § I.B (the paragraph in which footnote 9 is cited for the first time) as well as Eqs. (107), (108), (109) and (122) above), it follows that *no* finite-order perturbation theory (beyond the first order) for $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ in terms of the *bare* v can suffice in cases where $v \equiv v_c$ and $d = 3$. To be explicit, depending on whether $n_{\bar{\sigma}}(\boldsymbol{r}) - n_{\sigma}(\boldsymbol{r}) \not\equiv 0$ or $n_{\bar{\sigma}}(\boldsymbol{r}) - n_{\sigma}(\boldsymbol{r}) \equiv 0$, (*cf.* Eq. (G15)), such perturbation series involves unbounded contributions already at respectively the second or third order in the perturbation theory (see Eq. (129) above) when $v \equiv v_c$ in $d = 3$. To appreciate this point, suppose that, in contradiction to our assertion, a pth-order perturbation theory of the type mentioned would suffice, with $p > 2$ (let us say, for a system with an insulating GS). In such an event, $\Sigma_{\sigma;\infty_{p-1}}(\boldsymbol{r},\boldsymbol{r}')$ would have to be integrable and bounded almost everywhere (*cf.* conditions (A), (B) and (C) in § II.B), which our considerations in this Section show not to be the case when $p = 3$.

To complete our above arguments, it remains to consider the following observation: the many-body perturbation theory for $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ to which we have referred above, is one in terms of the *exact* single-particle GF G_{σ} and the *bare* particle-particle interaction function v, diagrammatically represented by means of skeleton diagrams (Luttinger and Ward 1960). Since G_{σ} is an implicit functional of v, depending on v to infinite order, it follows that the contribution of any single skeleton diagram to $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ is in fact non-perturbative. Consequently, the question may arise concerning relevance, if not validity, of our above assertion, in its general form, with regard to *finite*-order perturbation series for $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ in cases corresponding to $v \equiv v_c$ and $d = 3$. This question is readily dealt with, unequivocally establishing the validity of our above assertion, by considering the fact that the unbounded and non-integrable contributions to $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, with $m \geq 2$, remain (a fact that can be explicitly verified in the case when $m = 2$) by replacing the exact functions n_{σ}, ϱ_{σ}, $\Gamma^{(m)}$, in the pertinent expressions by their counterparts within the framework of the SSDA. In doing so it is important that the underlying single Slater determinant (SSD) (see Appendix C), namely $|\Phi_{N;0}\rangle$, is the GS of an $\widehat{H}_0$ with which the exact GS $|\Psi_{N;0}\rangle$ is adiabatically connected (see the paragraph preceding that containing Eq. (62)). To appreciate this aspect, consider the case where $n_{\sigma}(\boldsymbol{r}) \not\equiv n_{\bar{\sigma}}(\boldsymbol{r})$ so that $\widetilde{\mathsf{T}}^{\rm s}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}\|z) \not\equiv 0$ (see Eq. (G15)); evidently, to an inappropriate $|\Phi_{N;0}\rangle$, for which $n_{{\rm s};\sigma}(\boldsymbol{r}) \equiv n_{{\rm s};\bar{\sigma}}(\boldsymbol{r})$, corresponds an identically-vanishing $\widetilde{\mathsf{T}}^{\rm s}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}\|z)|_{\rm s}$.

I. The asymptotic series of the imaginary part of the self-energy for $|\varepsilon| \to \infty$

1. General considerations

In the earlier Sections we have dealt with the AS of the *full* SE for large values of $|\varepsilon|$. As we have emphasized (see § III.C), unless the entire series, or at least an *infinite* subset of its terms, is summed, a finite-order AS for $\Sigma_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ *cannot* but be real valued (see also the second paragraph in Appendix B). Here we deduce a finite-order large-$|\varepsilon|$ AS for $\mathrm{Im}\Sigma_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ which in conjunction with a finite-order AS for $\mathrm{Re}\Sigma_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, coinciding with that for $\Sigma_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, provide to some finite order in $1/\varepsilon$ the *complete* asymptotic behaviour of $\Sigma_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ for $|\varepsilon| \to \infty$. For a concise notation, in this Sections we denote $\Sigma_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ and related *functions*, such as $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, by $\Sigma_{\sigma}(\varepsilon)$ and $\Sigma_{\sigma;\infty_m}$ respectively; thus below $\Sigma_{\sigma}(\varepsilon)$ (and $\Sigma_{\sigma;\infty_m}$, etc.) should *not* be identified with the SE *operator*, but with its coordinate representation, which is a *function*.

The imaginary part of $\Sigma_\sigma(\varepsilon) \equiv \widetilde{\Sigma}_\sigma(\varepsilon \pm i\eta)$, $\varepsilon \gtrless \mu$, $\eta \downarrow 0$, is obtained in terms of its real part from the following Kramers-Krönig relation

$$\mathrm{Im}\widetilde{\Sigma}_\sigma(\varepsilon \pm i\eta) = \frac{\pm 1}{\pi}\,\mathrm{sgn}(\mu-\varepsilon)\,S_\sigma(\varepsilon), \quad \eta \downarrow 0, \qquad (217)$$

where

$$S_\sigma(\varepsilon) := \wp\int_{-\infty}^{\infty} \mathrm{d}\varepsilon'\;\frac{\mathrm{Re}\Sigma_\sigma(\varepsilon') - \Sigma_{\sigma;\infty_0}}{\varepsilon'-\varepsilon}. \qquad (218)$$

In Eq. (217), μ stands for the 'chemical potential' introduced in Eq. (22) above. Separating the interval of ε' integration into $(-\infty,0]$ and $[0,\infty)$ and employing the variable transformation $\varepsilon' \rightharpoonup -\varepsilon'$ in the first integral followed by the variable transformation $\varepsilon' \rightharpoonup 1/\varepsilon'$ in the integral thus obtained as well as the second integral, we arrive at

$$S_\sigma(\varepsilon) = \varepsilon\,\wp\int_0^{\infty} \mathrm{d}\varepsilon'\;\Big[(1+1/[\varepsilon\varepsilon'])\,\mathrm{Re}\Sigma_\sigma(1/\varepsilon') + (1-1/[\varepsilon\varepsilon'])\,\mathrm{Re}\Sigma_\sigma(-1/\varepsilon') - 2\Sigma_{\sigma;\infty_0}\Big]\big/\big(1-{\varepsilon'}^2\varepsilon^2\big). \qquad (219)$$

Now we decompose the interval of the ε' integration in Eq. (219) into $[0,\Delta]$ and $[\Delta,\infty)$, where Δ is some positive small number; later we shall assume $\Delta > 1/|\varepsilon|$ when $|\varepsilon| \to \infty$; we denote the former integral by $S_\sigma^{(1)}(\varepsilon)$ and the latter by $S_\sigma^{(2)}(\varepsilon)$. In dealing with the integral over $[0,\Delta]$, we employ (*cf.* Eq. (72) and see Eq. (62) above)

$$\Sigma_\sigma(\pm 1/\varepsilon') = \sum_{m=0}^{\infty} (\pm 1)^m\,\Sigma_{\sigma;\infty_m}\,{\varepsilon'}^m, \qquad (220)$$

from which, after some algebra, we obtain

$$(1+1/[\varepsilon\varepsilon'])\Sigma_\sigma(1/\varepsilon') + (1-1/[\varepsilon\varepsilon'])\Sigma_\sigma(-1/\varepsilon') - 2\Sigma_{\sigma;\infty_0} = \frac{2}{\varepsilon}\Sigma_{\sigma;\infty_1} + 2\sum_{m=1}^{\infty}\big[\Sigma_{\sigma;\infty_{2m}} + \frac{1}{\varepsilon}\Sigma_{\sigma;\infty_{2m+1}}\big]{\varepsilon'}^{2m}. \qquad (221)$$

Formally, the RHS of Eq. (221) is real valued for real values of ε'. Substituting this expression in the integral on the RHS of Eq. (219) with the interval of the ε' integration restricted to $[0,\Delta]$, we encounter the following two standard integrals

$$\wp\int_0^{\Delta} \mathrm{d}\varepsilon'\;\frac{1}{1-{\varepsilon'}^2\varepsilon^2} = \frac{1}{\varepsilon}\tanh^{-1}(1/[\Delta\varepsilon]) = \frac{1}{\Delta\,\varepsilon^2} + \mathcal{O}(1/\varepsilon^4), \qquad (222)$$

$$\wp\int_0^{\Delta} \mathrm{d}\varepsilon'\;\frac{{\varepsilon'}^{2m}}{1-{\varepsilon'}^2\varepsilon^2} = \frac{-\Delta^{2m-1}}{(2m-1)\varepsilon^2} \times {}_2F_1\big(1/2-m,1;3/2-m;1/[\Delta^2\varepsilon^2]\big) = -\frac{\Delta^{2m-1}}{(2m-1)\varepsilon^2} + \mathcal{O}(1/\varepsilon^4), \qquad (223)$$

where $\tanh^{-1}(x) \equiv \mathrm{arctanh}(x)$ stands for the inverse of $\tanh(x)$ and ${}_2F_1(a,b;c;x)$ for the generalized Gauss hypergeometric function (Abramowitz and Stegun 1972, p. 556). From the above results it immediately follows that

$$S_\sigma^{(1)}(\varepsilon) = \big[-2\sum_{m=1}^{\infty}\Sigma_{\sigma;\infty_{2m}}\,\frac{\Delta^{2m-1}}{2m-1}\big]\,\frac{1}{\varepsilon} + \big[\frac{2\Sigma_{\sigma;\infty_1}}{\Delta} - 2\sum_{m=1}^{\infty}\Sigma_{\sigma;\infty_{2m+1}}\,\frac{\Delta^{2m-1}}{2m-1}\big]\,\frac{1}{\varepsilon^2} + \mathcal{O}(\frac{1}{\varepsilon^3}). \qquad (224)$$

We note in passing that $\sum_{m=1}^{\infty}\Delta^{2m-1}/(2m-1) = \mathrm{arctanh}(\Delta)$.

Further, it is easily verified that

$$S_\sigma^{(2)}(\varepsilon) = -\frac{1}{\varepsilon}\,\wp\int_{\Delta}^{\infty}\frac{\mathrm{d}\varepsilon'}{{\varepsilon'}^2}\;\frac{\mathrm{Re}\Sigma_\sigma(1/\varepsilon') + \mathrm{Re}\Sigma_\sigma(-1/\varepsilon') - 2\Sigma_{\sigma;\infty_0}}{1-1/[{\varepsilon'}^2\varepsilon^2]} - \frac{1}{\varepsilon^2}\,\wp\int_{\Delta}^{\infty}\frac{\mathrm{d}\varepsilon'}{{\varepsilon'}^3}\;\frac{\mathrm{Re}\Sigma_\sigma(1/\varepsilon') - \mathrm{Re}\Sigma_\sigma(-1/\varepsilon')}{1-1/[{\varepsilon'}^2\varepsilon^2]}. \qquad (225)$$

For $|\varepsilon| > 1/\Delta$, taking into account that, in Eq. (225) $\varepsilon' \geq \Delta$, we can employ in the RHS of Eq. (225) the uniformly convergent series $1/(1-1/[{\varepsilon'}^2\varepsilon^2]) = \sum_{m=0}^{\infty}(1/[{\varepsilon'}^2\varepsilon^2])^m$ and thus obtain a uniformly convergent series in powers of $1/\varepsilon$, which amounts to the large-$|\varepsilon|$ AS for $S_\sigma^{(2)}(\varepsilon)$. Combining the result thus obtained for $S_\sigma^{(2)}(\varepsilon)$ and that for $S_\sigma^{(1)}(\varepsilon)$ in Eq. (224), we arrive at

$$S_\sigma(\varepsilon) = \Big[-2\sum_{m=1}^{\infty}\Sigma_{\sigma;\infty_{2m}}\,\frac{\Delta^{2m-1}}{2m-1} - \wp\int_{\Delta}^{\infty}\frac{\mathrm{d}\varepsilon'}{{\varepsilon'}^2}\;\big(\mathrm{Re}\Sigma_\sigma(1/\varepsilon') + \mathrm{Re}\Sigma_\sigma(-1/\varepsilon') - 2\Sigma_{\sigma;\infty_0}\big)\Big]\,\frac{1}{\varepsilon} + \Big[\frac{2\Sigma_{\sigma;\infty_1}}{\Delta} - 2\sum_{m=1}^{\infty}\Sigma_{\sigma;\infty_{2m+1}}\,\frac{\Delta^{2m-1}}{2m-1} - \wp\int_{\Delta}^{\infty}\frac{\mathrm{d}\varepsilon'}{{\varepsilon'}^3}\;\big(\mathrm{Re}\Sigma_\sigma(1/\varepsilon') - \mathrm{Re}\Sigma_\sigma(-1/\varepsilon')\big)\Big]\,\frac{1}{\varepsilon^2} + \mathcal{O}(\frac{1}{\varepsilon^3}), \quad \text{for } |\varepsilon| > 1/\Delta. \qquad (226)$$

One can readily verify that the derivatives with respect to Δ of the coefficients of the $1/\varepsilon$ and $1/\varepsilon^2$ terms on the RHS of Eq. (226) are *identically* vanishing, appropriately reflecting the fact that Δ does not appear in the defining expression for $S_\sigma(\varepsilon)$. We note that the *exact* Δ independence of the coefficients in the series in Eq. (226) is a direct consequence of taking *full* account of the series involving $\{\Sigma_{\sigma;\infty_{2m}}\}$ and $\{\Sigma_{\sigma;\infty_{2m+1}}\}$; truncation of these series at some finite order will result in the violation of this exact property. The magnitude of the error thus introduced can be made arbitrary small by reducing Δ, leading, however, through the condition $|\varepsilon| > 1/\Delta$ to the requirement that the corresponding expression for $S_\sigma(\varepsilon)$ be taken as accurate for increasingly larger values of $|\varepsilon|$.

We point out that, according to the asymptotic results obtained in the present work for $\mathrm{Re}\Sigma_\sigma(\varepsilon)$, we have $\mathrm{Re}\Sigma_\sigma(1/\varepsilon') + \mathrm{Re}\Sigma_\sigma(-1/\varepsilon') - 2\Sigma_{\sigma;\infty_0} = o(\varepsilon')$ for $\varepsilon' \to 0$, where $f(x) = o\big(g(x)\big)$ denotes the property $f(x)/g(x) \to 0$ for $x \to 0$. As a result of this fact, we observe that the first integral over ε' on the RHS of Eq. (226) is bounded for $\Delta \downarrow 0$. Consequently, insofar as the coefficient of the $1/\varepsilon$ on the RHS of Eq. (226) is concerned, we can set herein Δ equal to zero, which leads to the disappearance of the infinite sum in the expression for this coefficient. We cannot, however, *directly* follow this procedure of setting Δ equal to zero in the coefficient of $1/\varepsilon^2$ on the RHS of Eq. (226).

From Eqs. (217) and (226), setting Δ in the expression for the coefficient of $1/\varepsilon$ on the RHS of Eq. (226) equal to zero, we finally obtain (see the second part of the *notes added in proof*)

$$\mathrm{Im}\widetilde{\Sigma}_\sigma(\varepsilon \pm i\eta) = \frac{\pm\mathrm{sgn}(\mu-\varepsilon)}{\pi} \times\Big\{ -\wp\!\int_0^\infty \frac{\mathrm{d}\varepsilon'}{\varepsilon'^2}\,\big(\mathrm{Re}\Sigma_\sigma(1/\varepsilon') + \mathrm{Re}\Sigma_\sigma(-1/\varepsilon') - 2\Sigma_{\sigma;\infty_0}\big)\,\frac{1}{\varepsilon} + \Big[\frac{2\Sigma_{\sigma;\infty_1}}{\Delta} - 2\sum_{m=1}^{\infty} \Sigma_{\sigma;\infty_{2m+1}}\,\frac{\Delta^{2m-1}}{2m-1} - \wp\!\int_\Delta^\infty \frac{\mathrm{d}\varepsilon'}{\varepsilon'^3}\,\big(\mathrm{Re}\Sigma_\sigma(1/\varepsilon') - \mathrm{Re}\Sigma_\sigma(-1/\varepsilon')\big)\Big]\frac{1}{\varepsilon^2} + \mathcal{O}(\frac{1}{\varepsilon^3})\Big\}, \quad \text{for}\;\; |\varepsilon| > 1/\Delta. \tag{227}$$

Now we discuss an important limitation of the expression in Eq. (227) in specific cases which we shall indicate below. As should be evident, the validity of the result in Eq. (227) vitally depends on the assumption concerning admissibility of exchanging orders of summation and integration, which assumption has been basic in enabling us *term by term* to integrate the series representation $\sum_{m=0}^{\infty} \Sigma_{\sigma;\infty_m}/\varepsilon^m$ for $\Sigma_\sigma(\varepsilon)$; the derivation of the expression for $S_\sigma^{(1)}(\varepsilon)$ in Eq. (224), which has directly resulted in the expression for $\mathrm{Im}\widetilde{\Sigma}_\sigma(\varepsilon \pm i\eta)$ in Eq. (227), crucially depends on the integral in Eq. (223). However, as we have observed in § III.H, *not* all terms contributing to $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, with $m \ge 2$, are well defined, [94] and that regularization of such contributions requires *infinite* summations over specific category of equally ill-defined contributions pertaining to $\Sigma_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ with $p > m$ (see § II.B). It is exactly owing to these ill-defined contributions that the aforementioned procedure of term-by-term integration fails, necessitating us to resort to such procedure as that employed in Appendices F and G, where we evaluate the regularized contributions explicitly for strictly complex z (which contributions we denote by $\widetilde{\Sigma}^{\mathrm{s}}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)$; see Eq. (110) above) and subsequently deduce the real and imaginary parts of $\Sigma^{\mathrm{s}}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|\varepsilon)$ through the substitution $z \rightharpoonup \varepsilon \pm i\eta$, with $\eta \downarrow 0$ (*cf.* Eq. (65) above).

We can summarize the above considerations as follows. In deducing a finite-order large-$|\varepsilon|$ AS for $\mathrm{Im}\Sigma_\sigma(\varepsilon)$, one should consider the following decomposition of the SE into 'regular' and 'singular' contributions (*cf.* Eq. (110) above; see also conditions (A)-(C) in § II.B)

$$\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z) \equiv \widetilde{\Sigma}^{\mathrm{r}\oplus\mathrm{s_b}}_\sigma(\boldsymbol{r},\boldsymbol{r}';z) + \widetilde{\Sigma}^{\mathrm{s}}_\sigma(\boldsymbol{r},\boldsymbol{r}';z). \tag{228}$$

The 'regular' together with 'singular but bounded (almost everywhere)' contribution $\widetilde{\Sigma}^{\mathrm{r}\oplus\mathrm{s_b}}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ is defined as being one that possesses the following (asymptotic) series expansion

$$\widetilde{\Sigma}^{\mathrm{r}\oplus\mathrm{s_b}}_\sigma(\boldsymbol{r},\boldsymbol{r}';z) \equiv \sum_{m=0}^{\infty} \frac{\Sigma^{\mathrm{r}}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}') + \Sigma^{\mathrm{s_b}}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')}{z^m}, \tag{229}$$

in which the constituent coefficient functions $\{\Sigma^{\mathrm{r}}_{\sigma;\infty_m}\}$ and $\{\Sigma^{\mathrm{s_b}}_{\sigma;\infty_m}\}$ are defined in § III.E.2; the infinite series in Eq. (229) is characterized by the property that its truncation to a finite number of terms results in a well-defined AS for $\widetilde{\Sigma}^{\mathrm{r}\oplus\mathrm{s_b}}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ corresponding to $|z| \to \infty$ (although, unless $\Sigma^{\mathrm{s_b}}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}') \equiv 0$ for *all* m taken into account, the resulting series is *not* necessarily suitable for calculating an associated finite-order AS for the momentum representation of $\widetilde{\Sigma}_\sigma(z)$ for $|z| \to \infty$). The 'singular' contribution $\widetilde{\Sigma}^{\mathrm{s}}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$, on the other hand, is defined as one that is neither 'regular' nor 'singular but bounded (almost everywhere)'; we have (see Eq. (112) above and footnote 71)

$$\widetilde{\Sigma}^{\mathrm{s}}_\sigma(\boldsymbol{r},\boldsymbol{r}';z) \equiv \sum_{m=2}^{\infty} \frac{\widetilde{\Sigma}^{\mathrm{s}}_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}'\|z)}{z^m}. \tag{230}$$

The AS in Eq. (227) applies to (*cf.* Eq. (65) above)

$$\Sigma^{\mathrm{r}\oplus\mathrm{s_b}}_\sigma(\varepsilon) \equiv \lim_{\eta\downarrow 0} \widetilde{\Sigma}^{\mathrm{r}\oplus\mathrm{s_b}}_\sigma(\varepsilon \pm i\eta), \quad \varepsilon \gtrless \mu, \tag{231}$$

with the provision that *all* the functions Σ_σ and $\Sigma_{\sigma;\infty_m}$ in Eq. (227) be accordingly replaced by $\Sigma^{\mathrm{r}\oplus\mathrm{s_b}}_\sigma$ and $\Sigma^{\mathrm{r}}_{\sigma;\infty_m} + \Sigma^{\mathrm{s_b}}_{\sigma;\infty_m}$ respectively. In this connection, it is most relevant to realize that within the confines of our considerations in this paper, where we specifically focus on the peculiarities of v_c in $d = 3$ (see footnote 71), the leading-order contribution to the large-$|\varepsilon|$ AS for $\mathrm{Im}\Sigma^{\mathrm{s}}_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$

[94] We point out that here $m = 2$ is specific to systems in $d = 3$ with particles interacting through the Coulomb potential v_c. Thus $m = 2$ is *not* a universal number in the context of our present work.

is *sub-dominant* in comparison with $1/\varepsilon$, so that the Σ_σ functions in the coefficient of the $1/\varepsilon$ on the RHS of Eq. (227), remain the *complete* functions, as opposed to their 'regular' and 'singular but bounded' parts. [95]

Determination of $\mathrm{Im}\Sigma_\sigma^{\mathrm{s}}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, on the other hand, should either proceed from Eqs. (217) and (218), with the provision that *all* the Σ_σ functions herein be replaced by $\Sigma_\sigma^{\mathrm{s}}$, or from an explicitly evaluated $\widetilde{\Sigma}_\sigma^{\mathrm{s}}(z)$ by means of an appropriate analytic continuation of the latter function on to the real ε-axis (see Appendices F, G and H; see also Eqs. (F161), (G17) and (H21)). Note that, since in all cases $\Sigma_{\sigma;\infty_0}$ is regular, so that we have $\Sigma_{\sigma;\infty_0}^{\mathrm{r}} \equiv \Sigma_{\sigma;\infty_0}$, it follows that $\Sigma_{\sigma;\infty_0}^{\mathrm{s_b}} \equiv 0$ and $\widetilde{\Sigma}_{\sigma;\infty_0}^{\mathrm{s}} \equiv 0$. Thus, in employing Eqs. (217) and (218), while dealing with $\Sigma_\sigma^{\mathrm{s}}(\varepsilon)$, we have *no* ε-*in*dependent contribution on the RHS of Eq. (218). Note further that $\widetilde{\Sigma}_\sigma^{\mathrm{s}}(z)$ may be identically vanishing, as is the case for systems of fermions interacting through bounded and short-range v.

Finally, we point out that the relevance of the expression in Eq. (227) is largely conceptual rather than necessarily practical; as is evident from the ε' integrals on the RHS of Eq. (227), which together cover the interval $[0,\infty)$, the mere knowledge of a finite-order AS for $\mathrm{Re}\Sigma_\sigma(\varepsilon)$ (read $\mathrm{Re}\Sigma_\sigma^{\mathrm{r}\oplus\mathrm{s_b}}(\varepsilon)$) corresponding to $|\varepsilon| \to \infty$ is *not* sufficient for the purpose of determining $\mathrm{Im}\Sigma_\sigma(\varepsilon)$ (read $\mathrm{Im}\Sigma_\sigma^{\mathrm{r}\oplus\mathrm{s_b}}(\varepsilon)$) at large values of $|\varepsilon|$. Below we shall encounter an instance where the conceptual relevance of the result in Eq. (227) becomes fully apparent.

2. *Uniform isotropic systems; the single-particle spectral function $\overline{A}_\sigma(k;\varepsilon)$*

Here we determine some leading-order terms in the large-$|\varepsilon|$ AS of the single-particle spectral function $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ pertaining to a uniform and isotropic system. Consequently, here as in § III.E we employ the notation $k{:=}\|\boldsymbol{k}\|$. The uniformity of the system entails that the Dyson equation, which is an integral equation in the coordinate representation, reduces to an algebraic equation in the momentum representation; we have

$$\widetilde{\overline{G}}_\sigma(k;z) = \widetilde{\overline{G}}_{0;\sigma}(k;z) + \widetilde{\overline{G}}_{0;\sigma}(k;z)\widetilde{\overline{\Sigma}}_\sigma^{\sharp}(k;z)\widetilde{\overline{G}}_\sigma(k;z), \tag{232}$$

where $\widetilde{\Sigma}_\sigma^{\sharp}$ is defined in Eq. (62); since the constant external potential to which fermions are exposed is independent of σ, it is the dependence on σ of the GF pertaining to the 'non-interacting' system, i.e. $\widetilde{\overline{G}}_{0;\sigma}(k;z)$, that has necessitated introduction in Eq. (232) of $\widetilde{\Sigma}_\sigma^{\sharp}(z)$ in place of $\widetilde{\Sigma}_\sigma(z)$ (see § III.C). [96] The isotropy of the system together with our specific choice of gauge (see Appendix B) imply that the real and imaginary parts of the functions in Eq. (232) are the Fourier transforms of the real and imaginary parts respectively of their real-space counterparts. In other words, the result in Eq. (227) which, as we have clearly stated at the outset of § III.I.1, is applicable to $\mathrm{Im}[\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)]$, also applies to $\mathrm{Im}[\overline{\Sigma}_\sigma(k;\varepsilon)] \equiv \mathrm{Im}[\overline{\Sigma}_\sigma^{\sharp}(k;\varepsilon)]$. The same is the case concerning $\mathrm{Re}[\overline{\Sigma}_\sigma(k;\varepsilon)]$, that is we can employ the result in Eq. (112), with $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')$, $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$, ... herein replaced by $\overline{\Sigma}_{\sigma;\infty_0}(k)$, $\overline{\Sigma}_{\sigma;\infty_1}(k)$, ... For our discussions that follow, for $|\varepsilon| \to \infty$ we thus write

$$\mathrm{Re}\overline{\Sigma}_\sigma(k;\varepsilon) \sim \overline{\Sigma}_{\sigma;\infty_0}(k) + \frac{\overline{\Sigma}_{\sigma;\infty_1}(k)}{\varepsilon}, \tag{233}$$

$$\mathrm{Im}\widetilde{\overline{\Sigma}}_\sigma(k;\varepsilon \pm i\eta) \sim \frac{\pm\mathrm{sgn}(\mu-\varepsilon)}{\pi} \times \begin{cases} \dfrac{\overline{\Xi}_\sigma(k)}{\varepsilon} + \dfrac{\overline{\Pi}_\sigma(k)}{\varepsilon^2}, & \text{(I)} \\[2ex] \dfrac{\overline{\Xi}_\sigma(k)}{\varepsilon} - 4\pi^2\big(\dfrac{e^2}{4\pi\epsilon_0}\big)^2 \dfrac{(n_{0;\bar{\sigma}} - n_{0;\sigma})}{\sqrt{2m_e}}\, \dfrac{\Theta(\varepsilon-\mu)}{\varepsilon^{3/2}} \\[2ex] \quad + \dfrac{\overline{\Pi}_\sigma(k) - 4\pi^3\hbar^{-1}(e^2/[4\pi\epsilon_0])^3 n_{0;\bar{\sigma}}\,\Theta(\varepsilon-\mu)}{\varepsilon^2}, & \text{(II)} \end{cases} \tag{234}$$

where $\overline{\Xi}_\sigma(k)$ and $\overline{\Pi}_\sigma(k)$ stand for the diagonal elements of the spatial Fourier transforms with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$ of the coefficients of $1/\varepsilon$ and $1/\varepsilon^2$ on the RHS of Eq. (227). In Eq. (234), (I) corresponds to $v \not\equiv v_c$ and (II) to $v \equiv v_c$ in $d = 3$. Note that depending on whether $v \not\equiv v_c$ or $v \equiv v_c$, $\Xi_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and $\Pi_\sigma(\boldsymbol{r},\boldsymbol{r}')$, and consequently $\overline{\Xi}_\sigma(k)$ and $\overline{\Pi}_\sigma(k)$, are, as clearly specified in the text following Eq. (227), slightly different functions. From Eq. (234) we observe that for $\varepsilon \to -\infty$ ('photo-emission'), $\mathrm{Im}\overline{\Sigma}_\sigma(k;\varepsilon)$ corresponding to the cases (I) and (II) have identical

[95] This aspect, which is reflected in the lower bound of the summation on the RHS of Eq. (230), is implicit in the considerations preceding Eq. (227) which led to the possibility of identifying Δ in the first term on the RHS of Eq. (226) with zero. In this connection we point out that our above conclusion with regard to the leading-order contribution in the large-$|\varepsilon|$ AS for $\mathrm{Im}\Sigma_\sigma(\varepsilon)$ is fully borne out by our explicit calculations in § III.I.1. Following our brief references in footnote 12 and in the text following Eq. (112) to systems of fermions confined to $d = 2$ and interacting through $v \equiv v_c$, we note that the leading-order contribution to the large-$|\varepsilon|$ AS for $\mathrm{Im}\Sigma_\sigma^{\mathrm{s}}(\varepsilon)$ pertaining to these systems is asymptotically more dominant than $1/\varepsilon$ (B. Farid, 2001, unpublished).

[96] By choosing the 'non-interacting' GF to be that pertaining to $h_{0;\sigma}(\boldsymbol{r})$ (see Eq. (55)) (with $u(\boldsymbol{r})$ a constant), rather than $h_0(\boldsymbol{r})$ (see Eq. (43)), we are capable of dealing with (homogeneous) magnetic GSs.

functional forms and that, for $\varepsilon \to +\infty$ ('inverse-photo-emission'), $\mathrm{Im}\overline{\Sigma}_\sigma(k;\varepsilon)$ corresponding to cases (I) and (II) are fundamentally different especially when $n_{0;\bar{\sigma}} \neq n_{0;\sigma}$. For clarity, $n_{0;\bar{\sigma}}$ (note the $\bar{\sigma}$, the complement of σ) in the last term on the RHS of Eq. (234), entry (II), has its origin in the combination of two contributions: one being $\hbar^{-1}\mathsf{M}^{\mathrm{s}}_{\infty_2}(\boldsymbol{r}\|z)\,\delta(\boldsymbol{r}-\boldsymbol{r}')$ (see Eqs. (213), (F160) and (F161)) which depends on n (the *total* number density), and the other $\widetilde{\Sigma}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}';z)$ (see Eqs. (212), (H2) and (H21)) which depends on n_σ. We note in passing that the requirement for the stability of the GS (see § III.D) implies that $\overline{\Xi}_\sigma(k) \geq 0, \forall\, k, \sigma$.

From Eq. (55), making use of

$$\widetilde{\overline{G}}_{0;\sigma}(k;z) = \frac{\hbar}{z - \bar{h}_{0;\sigma}(k)}, \tag{235}$$

with $\bar{h}_{0;\sigma}(k)$ the Fourier transform of $h_{0;\sigma}(\boldsymbol{r})$ as defined in Eq. (55) above, one immediately obtains

$$\widetilde{\overline{G}}_\sigma(k;z) = \frac{\hbar}{z - [\bar{h}_0(k) + \hbar\widetilde{\overline{\Sigma}}_\sigma(k;z)]}, \tag{236}$$

where $\bar{h}_0(k)$ denotes the Fourier transform of $h_0(\boldsymbol{r})$ as defined in Eq. (43) above. From Eq. (236) and the definition in Eq. (39), we have

$$\overline{A}_\sigma(k;\varepsilon) = \frac{\hbar}{\pi} \times \frac{\hbar|\mathrm{Im}\overline{\Sigma}_\sigma(k;\varepsilon)|}{\big(\varepsilon - [\bar{h}_0(k) + \hbar\mathrm{Re}\overline{\Sigma}_\sigma(k;\varepsilon)]\big)^2 + \big(\hbar\mathrm{Im}\overline{\Sigma}_\sigma(k;\varepsilon)\big)^2}. \tag{237}$$

In arriving at this result, we have made use of the fact that

$$\widetilde{\overline{\Sigma}}_\sigma(k;\varepsilon \pm i\eta) = \mathrm{Re}\overline{\Sigma}_\sigma(k;\varepsilon) \mp i|\mathrm{Im}\overline{\Sigma}_\sigma(k;\varepsilon)|, \;\; \eta \downarrow 0, \tag{238}$$

where $\overline{\Sigma}_\sigma(k;\varepsilon)$ stands for the *physical* SE (see Eq. (65) above). Making use of the results in Eqs. (233) and (234), from Eq. (237) for $|\varepsilon| \to \infty$ we immediately deduce that

$$\overline{A}_\sigma(k;\varepsilon) \sim \frac{\hbar^2}{\pi^2}\,\frac{\mathrm{sgn}(\varepsilon-\mu)}{\varepsilon^3} \times \begin{cases} \overline{\Xi}_\sigma(k) + \dfrac{2\big(\bar{h}_0(k) + \hbar\overline{\Sigma}_{\sigma;\infty_0}(k)\big)\,\overline{\Xi}_\sigma(k) + \overline{\Pi}_\sigma(k)}{\varepsilon}, & \text{(I)} \\[2ex] \overline{\Xi}_\sigma(k) - 4\pi^2\big(\dfrac{e^2}{4\pi\epsilon_0}\big)^2\,\dfrac{(n_{0;\bar{\sigma}} - n_{0;\sigma})}{\sqrt{2m_e}}\,\dfrac{\Theta(\varepsilon-\mu)}{\varepsilon^{1/2}} \\ \quad + \big[2\big(\bar{h}_0(k) + \hbar\overline{\Sigma}_{\sigma;\infty_0}(k)\big)\,\overline{\Xi}_\sigma(k) + \overline{\Pi}_\sigma(k) \\ \quad -4\pi^3\hbar^{-1}(e^2/[4\pi\epsilon_0])^3\, n_{0;\bar{\sigma}}\,\Theta(\varepsilon-\mu)\big]/\varepsilon. & \text{(II)} \end{cases} \tag{239}$$

By Fourier transforming both sides of Eq. (239) back to the $(\boldsymbol{r},\boldsymbol{r}')$-space, one arrives at the result that, for the uniform isotropic system under consideration, the large-$|\varepsilon|$ asymptotic behaviour of $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (more precisely, $A^{\mathrm{h}}_\sigma(\|\boldsymbol{r}-\boldsymbol{r}'\|;\varepsilon)$; see Eq. (F9)) is similar to that of $\overline{A}_\sigma(k;\varepsilon)$ in Eq. (239). The results in Eq. (239) are specifically significant in revealing that for the uniform and isotropic system under consideration, the energy moments of $\overline{A}_\sigma(k;\varepsilon)$, or of $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, are *not* bounded for $m \geq 3$ (see Eqs. (37) and (38) above as well as footnote 6). It is important to point out that, following the specification in Eq. (37), $\overline{G}_{\sigma;\infty_m}(k)$ is bounded for $m = 3$; whereas the leading term in the AS for the integrand of the ε integral on the RHS of Eq. (38) decays like $1/\varepsilon$ for large values of $|\varepsilon|$, the integral over $(-E,E)$ has a well-defined limit for $E \to \infty$, following the fact that $1/\varepsilon$ is an *odd* function of ε.

The expression in Eq. (239) in particular exposes some significant aspects of the (angle-resolved) photo-emission and inverse-photo-emission data and the way in which the latter are considerably affected through an imbalance between $n_{0;\bar{\sigma}}$ and $n_{0;\sigma}$. We should emphasize that the result in Eq. (239) is *strictly* only valid for uniform and isotropic systems and that, for other systems, the behaviour of the single-particle spectral function is *not* as simple and transparent as that in Eq. (239). We postpone considerations concerning $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ and $\overline{\overline{A}}_\sigma(\boldsymbol{k},\boldsymbol{k}';\varepsilon)$ as appropriate to inhomogeneous systems to a future publication. Suffice it for the moment to mention that even a small amount of inhomogeneity is capable of bringing about *considerable* change in the behaviour of the single-particle spectral function in comparison with that in the expression in Eq. (239).

Finally, we point out that the dependence on ε of $\overline{A}_\sigma(k;\varepsilon)$ pertaining to uniform and isotropic systems of Coulomb-interacting fermions confined to d-dimensional space with $d \neq 3$, in particular with $d = 2$ (B. Farid, 2001, unpublished) (see footnote 12), is so distinctly different from that of $\overline{A}_\sigma(k;\varepsilon)$ in Eq. (239) (corresponding to $d = 3$) that it suggests the feasibility of an experimental determination of the (effective) dimension of the space to which fermions are confined, through investigating the ε dependence of the corresponding single-particle spectral functions.

IV. CONVENTIONAL PERTURBATION THEORY AND THE CASE OF DYNAMICALLY SCREENED EXCHANGE SELF-ENERGY OPERATOR $\Sigma'^{(1)}_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$

The dynamically screened exchange SE operator is the first-order contribution to (see Eq. (62) above)

$$\Sigma'_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon) := \Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon) - \frac{1}{\hbar}v_H(\boldsymbol{r};[n])\,\delta(\boldsymbol{r}-\boldsymbol{r}')$$

$$\equiv \Sigma_\sigma^\sharp(\boldsymbol{r},\boldsymbol{r}';\varepsilon) + \frac{1}{\hbar}\big(w_\sigma(\boldsymbol{r}) - v_H(\boldsymbol{r};[n])\big)\,\delta(\boldsymbol{r}-\boldsymbol{r}') \quad (240)$$

in the perturbation series expansion of this function (see § III.C) in terms of the dynamically-screened particle-particle interaction function $W(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (Hubbard 1957) which in contrast with the bare particle-particle interaction $v(\boldsymbol{r}-\boldsymbol{r}')$ is a function of both $\boldsymbol{r}$ and $\boldsymbol{r}'$, rather than merely $\|\boldsymbol{r}-\boldsymbol{r}'\|$ (leaving aside the case of uniform and isotropic systems), and a function of the external energy parameter ε; in Eq. (240), n in the argument of $v_H(\boldsymbol{r};[n])$ (see Eq. (14) above) is the total GS number density pertaining to the interacting system.

It is well known, in particular for systems with metallic GSs (for example Mattuck (1992, § 10.4)), that the perturbation series for $\Sigma_\sigma(\varepsilon)$ in terms of v involves unbounded contributions when (not exclusively) $v \equiv v_c$ in $d = 3$, associated with integrals that owing to the long range of the Coulomb potential are infrared divergent. These unbounded contributions can be traced back as arising from the polarization insertions that collectively constitute the random-phase approximation (RPA) to the polarization function; the *total* contribution of the RPA series to the polarization function modifies the behaviour of the corresponding $W(\boldsymbol{r},\boldsymbol{r}';\varepsilon = 0)$ for $\|\boldsymbol{r}-\boldsymbol{r}'\| \to \infty$, in comparison with that of $v_c(\boldsymbol{r}-\boldsymbol{r}')$, in such a way [97] that substitution of $W^{\rm RPA}(\varepsilon)$ (or in a further approximation, of $W^{\rm RPA}(\varepsilon = 0)$) for $W(\varepsilon)$ in the perturbation series for $\Sigma_\sigma(\varepsilon)$ in terms of this function, results in a series that is free from the aforementioned unbounded contributions. The conventional wisdom concerning this subject (for example Mattuck (1992, § 10.4)) is that for non-metallic systems (i.e. those whose low-lying single-particle excitation spectrum is fully gapped) the above-mentioned unbounded contributions do *not* occur, so that for these systems the many-body perturbation series for $\Sigma_\sigma(\varepsilon)$ in terms of v_c does *not* contain unbounded contributions. Our considerations in § III.H.2 have unequivocally shown that this viewpoint is *not* correct (see in particular the last two paragraphs in § III.H.2). [98] This observation makes evident that, when choosing to employ a many-body perturbation series for $\Sigma_\sigma(\varepsilon)$, the series must be, in the cases corresponding to $v \equiv v_c$ in $d = 3$ (not exclusively), in terms of $W(\varepsilon)$ rather than v_c, independent of whether the GS of the system is metallic or otherwise.

Below we consider the expression for the first-order contribution to the perturbation series of $\Sigma'_\sigma(\varepsilon)$ in terms of $W(\varepsilon)$, as deduced from that of $\Sigma_\sigma^\sharp(\varepsilon)$, and assume both $G_\sigma(\varepsilon)$ and $W(\varepsilon)$ herein to coincide with those pertaining to the interacting system; we denote this first-order term, or the 'screened-exchange' SE (also called the GW SE), by $\Sigma_\sigma^{\prime(1)}(\varepsilon)$. At places we also comment on the consequences of replacing $G_\sigma(\varepsilon)$ by $G_{0;\sigma}(\varepsilon)$ (pertaining to the 'non-interacting' system corresponding to $\widehat{H}_0$ in Eq. (54)) and $W(\varepsilon)$ by $W^{\rm RPA}(\varepsilon)$; the latter function can in turn be one evaluated in terms of either $G_\sigma(\varepsilon)$ or $G_{0;\sigma}(\varepsilon)$.

For the first-order, or the screened-exchange, SE we have

$$\Sigma_\sigma^{\prime(1)}(\boldsymbol{r},\boldsymbol{r}';\varepsilon) = \frac{i}{\hbar}\int_{-\infty}^{\infty}\frac{{\rm d}\varepsilon'}{2\pi\hbar}\, G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon-\varepsilon') \times W(\boldsymbol{r},\boldsymbol{r}';\varepsilon')\,\exp(-i\varepsilon'\eta/\hbar),\;\; \eta\downarrow 0. \quad (241)$$

Later in this Section, we denote the SE $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ associated through Eq. (240) with $\Sigma_\sigma^{\prime(1)}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, by $\Sigma_\sigma^{(1)}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$. The screened interaction function can be written as

$$W(\boldsymbol{r},\boldsymbol{r}';\varepsilon) = v(\boldsymbol{r}-\boldsymbol{r}') + W'(\boldsymbol{r},\boldsymbol{r}';\varepsilon), \quad (242)$$

where $W'(\varepsilon)$ has the following Lehmann-type spectral representation

$$W'(\boldsymbol{r},\boldsymbol{r}';\varepsilon) = \sum_{s,\sigma} w_{s;\sigma}(\boldsymbol{r}) w_{s;\sigma}^*(\boldsymbol{r}') \times\Big\{\frac{1}{\varepsilon - e_s + i\eta} - \frac{1}{\varepsilon + e_s - i\eta}\Big\},\;\; \eta\downarrow 0, \quad (243)$$

where

[97] Previously (Farid 1999a, footnote 48) we have shown that for a uniform and isotropic system of spin-1/2 fermions in the paramagnetic state, for $\|\boldsymbol{r}\| \to \infty$ one has $W^{\rm RPA}(\|\boldsymbol{r}\|;0) \sim A\cos(2k_F\|\boldsymbol{r}\|)/\|\boldsymbol{r}\|^3$, where A stands for a constant and k_F for the Fermi wavenumber.

[98] Note that $\mathcal{M}(\boldsymbol{r})$ is a third-order contribution, whereas $\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})$ is a second-order one; this is particularly evident from the expression for $\mathsf{M}^{\rm s}_{\infty_2}(\boldsymbol{r}\|z)$ in Eq. (F160) where one observes $(e^2/[4\pi\epsilon_0])^3$ on the RHS and from the expression for $\widetilde{\mathsf{T}}^{\rm s}_{\sigma,\bar\sigma;\infty_2}(\boldsymbol{r}\|z)$ in Eq. (G15) where one observes $(e^2/[4\pi\epsilon_0])^2$ on the RHS. It is interesting to note that whereas the analysis as presented in Mattuck (1992) shows breakdown of perturbation theory in terms of v_c at the second order for metallic GSs, the second-order contribution $\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})$ is identically vanishing for $n_\sigma(\boldsymbol{r}) \equiv n_{\bar\sigma}(\boldsymbol{r})$ (see Eq. (129), from which it is evident that, for $n_{0;\sigma} = n_{0;\bar\sigma}$, the first transcendental function of r_s, namely $\ln(-\bar z/r_s^3)$, is pre-multiplied by r_s^3). This is a remarkable result in that the counterpart of $\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})$ within the framework of the first-order perturbation theory in terms of the dynamically screened interaction $W(\varepsilon)$, namely $\mathcal{T}^{(1)}(\boldsymbol{r})$ introduced in Eq. (278) below (an unbounded function in the case of $v \equiv v_c$ and $d = 3$), is *never* vanishing. For clarity, the stark contrast between $\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})$ and $\mathcal{T}^{(1)}(\boldsymbol{r})$ has its origin in the *incorrect* description of the non-local part of $\Sigma_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ by $\Sigma^{(1)}_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ for $p \ge 1$ (see the last two paragraphs in § III.H.2); for a correct reproduction of $\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})$ it is necessary also to consider the second-order skeleton SE diagrams in terms of v_c and the exact single-particle GF.

$$w_{s;\sigma}(\boldsymbol{r}) := \int \mathrm{d}^d r'\; v(\boldsymbol{r}-\boldsymbol{r}')\, \rho_{s;\sigma}(\boldsymbol{r}'), \tag{244}$$

with

$$\rho_{s;\sigma}(\boldsymbol{r}) := \langle \Psi_{N;0} | \hat{\psi}_\sigma^\dagger(\boldsymbol{r}) \hat{\psi}_\sigma(\boldsymbol{r}) - n_\sigma(\boldsymbol{r}) | \Psi_{N;s} \rangle, \tag{245}$$

so that $\rho_{0;\sigma}(\boldsymbol{r}) \equiv 0$, and

$$e_s := E_{N,s} - E_{N,0} \geq 0, \tag{246}$$

which are the energies of the *neutral* excitations of the N-particle system; the assumed non-degeneracy of the GS implies that $e_s > 0$ for *all* $s \neq 0$; as should be evident from $E_{N;0}$, here $s = 0$ symbolically denotes the N-particle GS of $\widehat{H}$. We point out that the compound variable s, $s \neq 0$, in the above expressions characterizes the excited $(N_\sigma + N_{\bar{\sigma}})$-particle eigenstates of $\widehat{H}$, so that for *interacting* systems it is a fundamentally different compound variable from that encountered in the Lehmann representation for $G_\sigma(\varepsilon)$ in Eq. (17) (and as subscript of the associated functions), where s characterizes the ground and excited $(N_\sigma \pm 1 + N_{\bar{\sigma}})$-particle eigenstates of $\widehat{H}$. When the two types of variable are encountered in the same expression (as in Eq. (251) below), each is uniquely identified through its association with functions that are known to have their origins in $G_\sigma(\varepsilon)$ (such as $\{f_{s;\sigma}(\boldsymbol{r})\}$) or $W(\varepsilon)$ (such as $\{w_{s;\sigma}(\boldsymbol{r})\}$).

Further, the apparent independence of $\{e_s\}$ on σ originates from the fact that $\{\hat{\psi}_\sigma^\dagger(\boldsymbol{r})\hat{\psi}_\sigma(\boldsymbol{r})\}$ commutes with $\{\widehat{N}_\sigma\}$, implying that $\hat{\psi}_\sigma^\dagger(\boldsymbol{r})\hat{\psi}_\sigma(\boldsymbol{r})$, $\forall\sigma$, has *vanishing* amplitude with respect to the ground and *any* excited N-particle state of $\widehat{H}$ whose N_σ, satisfying $N_\sigma + N_{\bar{\sigma}} = N$, differs from that pertaining to the GS. [99] This may be compared with the dependence upon σ of the single-particle excitation energies $\{\varepsilon_{s;\sigma}\}$, defined in Eq. (19), which has its root in the fact that $\{\hat{\psi}_\sigma(\boldsymbol{r})\}$ and $\{\hat{\psi}_\sigma^\dagger(\boldsymbol{r})\}$ do *not* commute with $\{\widehat{N}_\sigma\}$. With reference to our considerations in § III.F (see in particular footnote 87), we mention that, for exactly the same reasons that $\varepsilon = \mu_{N;\sigma}^{\mp}$ are accumulation points of the set of single-particle excitations energies, $\varepsilon = \lambda_N$, with $\lambda_N := \min\{e_s \| s \neq 0\}$, is an accumulation point of the set of neutral excitations energies of the N-particle system. Accordingly, $z = \pm\lambda_N$ are *non*-isolated singularities of $\widetilde{W}(z)$, analogous to $z = \mu_{N;\sigma}^{\mp}$ which are *non*-isolated singularities of $\widetilde{G}_\sigma(z)$ and $\widetilde{\Sigma}_\sigma(z)$. Further, similar to $[\mu_{N;\sigma}^{-}, \mu_{N;\sigma}^{+}]$ (see Eq. (22)), $[-\lambda_N, \lambda_N]$ can be infinitesimally small for systems in the thermodynamic limit, but it is never vanishing (see Eq. (246) above and the subsequent text).

For our later considerations, we introduce the analytic continuation into the physical Riemann sheet of $W'(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, namely (*cf.* Eq. (24) above and see footnote 11)

$$\widetilde{W}'(\boldsymbol{r},\boldsymbol{r}';z) = 2\sum_{s,\sigma} e_s\, \frac{w_{s;\sigma}(\boldsymbol{r}) w_{s;\sigma}^*(\boldsymbol{r}')}{z^2 - e_s^2}, \tag{247}$$

which is directly deduced from the representation in Eq. (243). The 'physical' $W'(\varepsilon)$ is obtained from $\widetilde{W}'(z)$ according to (*cf.* Eq. (25) above)

$$W'(\varepsilon) = \lim_{\eta\downarrow 0} \widetilde{W}'(\varepsilon \pm i\eta), \quad \varepsilon \gtrless 0. \tag{248}$$

From the expression in Eq. (247) we obtain the following series:

$$\widetilde{W}'(\boldsymbol{r},\boldsymbol{r}';z) = \sum_{m=1}^{\infty} \frac{W'_{\infty_{2m}}(\boldsymbol{r},\boldsymbol{r}')}{z^{2m}}, \tag{249}$$

where

$$W'_{\infty_m}(\boldsymbol{r},\boldsymbol{r}') := 2\sum_{s,\sigma} e_s^{m-1} w_{s;\sigma}(\boldsymbol{r}) w_{s;\sigma}^*(\boldsymbol{r}'). \tag{250}$$

The series in Eq. (249) is in all essential respects similar to that for $\widetilde{G}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ presented in Eq. (27). Thus, for instance, by truncating this series at some finite order, one obtains a *formal* finite-order AS (see § II.B) for $\widetilde{W}'(\boldsymbol{r},\boldsymbol{r}';z)$ corresponding to $|z| \to \infty$. Our explicit calculations of $W'_{\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ for $m = 1,2,3$ (see Eqs. (256), (264) and (273) respectively; note that, of these three functions, only the one corresponding to $m = 2$ is relevant to the large-$|z|$ AS for $\widetilde{W}'(\boldsymbol{r},\boldsymbol{r}';z)$) show that in the cases corresponding $v \equiv v_c$ in $d = 3$, these functions are *bounded* for $\boldsymbol{r} \neq \boldsymbol{r}'$; however, already for $m = 2$, $W'_{\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ diverges as $\|\boldsymbol{r}-\boldsymbol{r}'\| \to 0$. Since, in the expression for $\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ to be presented in Eq. (253) below, $W'_{\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ is multiplied by $\delta(\boldsymbol{r}-\boldsymbol{r}')$, the mentioned divergence of $W'_{\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ for $\boldsymbol{r} = \boldsymbol{r}'$ implies that,

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[99] The following two points are clarifying. First, the fact that to *all* orders of perturbation theory we merely encounter $W'(\varepsilon') \equiv \sum_{\sigma'} W'_{\sigma',\sigma'}(\varepsilon')$ (see Eqs. (241) and (242)) in the expression for $\Sigma_\sigma(\varepsilon)$, rather than $W'_{\sigma',\sigma''}(\varepsilon')$ followed by appropriate trace operations involving other functions of σ' and σ'', is to do with the assumed spin *independence* of v (for completeness, $W'_{\sigma',\sigma''}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ is defined in terms of $[\hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r})\hat{\psi}_{\sigma'}(\boldsymbol{r}) - n_{\sigma'}(\boldsymbol{r})]$ and $[\hat{\psi}_{\sigma''}^\dagger(\boldsymbol{r}')\hat{\psi}_{\sigma''}(\boldsymbol{r}') - n_{\sigma''}(\boldsymbol{r}')]$). Second, although e_s is independent of σ, its actual participation in the expression for $W'_{\sigma,\sigma}(\varepsilon)$ is determined by $w_{s;\sigma}$, or $\rho_{s;\sigma}$ (see Eq. (245)); thus although s is *independent* of σ, through the dependence on both s *and* σ of $w_{s;\sigma}$, s to the right of $\sum_s$ on the RHS of Eq. (243) can be considered as an *implicit* function of σ (one can of course equally consider σ in Eq. (243) to be an *implicit* function of s). This aspect is made evident through replacing the interacting states on the RHS of Eq. (245) by their 'non-interacting' counterparts (i.e. SSDs), whereon $W'(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ in Eq. (243) transforms into the leading-order term in the RPA series for this function; comparing this with the well-known RPA result for 'non-interacting' fermions, for these systems, one directly establishes the mentioned *implicit* dependence on σ of s.

similar to the $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$, $\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ is fundamentally unbounded in the case of $v \equiv v_c$ in $d=3$. With reference to the discussions in §§ II.B and III.H, it follows that, in the correct finite-order AS of $\widetilde{\Sigma}^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ for $|z|\to\infty$, the term decaying like $1/|z|$ is *not* directly followed by one decaying like $1/|z^2|$, rather by one or several asymptotically more dominant terms (see specifically Eqs. (277) and (278) below and the related discussions). In this work we do *not* discuss the details of these terms in much depth, in particular we do *not* give special attention to the case corresponding to $v\equiv v_c$ in $d=3$.

Before proceeding, we note in passing that, in contrast with $\widetilde{G}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$, which, according to the expression presented in Eq. (27), is determined by *all* $G_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, $\widetilde{W}'(\boldsymbol{r},\boldsymbol{r}';z)$, according to the expression in Eq. (249), is determined by a *proper* subset of all $W'_{\infty_m}(\boldsymbol{r},\boldsymbol{r}')$. Interestingly, as we shall see later (see Eqs. (253) - (255) below), the *entire* set $\big\{W'_{\infty_m}(\boldsymbol{r},\boldsymbol{r}')\big\}$ contributes to the large-$|z|$ AS for $\widetilde{\Sigma}^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$. We shall clarify the mechanism underlying this counter-intuitive and interesting phenomenon later in this Section.

From the Lehmann representation for $G_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ in Eq. (17), making use of the residue theorem and subsequently analytically continuing the resulting expression for (see Eq. (240) and compare with Eq. (62) above)

$$\Sigma^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)\equiv\Sigma^{\sharp(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)+\frac{1}{\hbar}w_{\sigma}(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}')$$

into the physical Riemann sheet, from the defining expression in Eq. (241) and from Eqs. (240) and (173) we obtain

$$\widetilde{\Sigma}^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)=\Sigma^{\rm HF}(\boldsymbol{r},\boldsymbol{r}';[\varrho_{\sigma}]) +\frac{1}{\hbar}\sum_{s,s'}\frac{f_{s;\sigma}(\boldsymbol{r})f^{*}_{s;\sigma}(\boldsymbol{r}')\sum_{\sigma'}w_{s';\sigma'}(\boldsymbol{r})w^{*}_{s';\sigma'}(\boldsymbol{r}')}{z-\varepsilon_{s;\sigma}-\mathrm{sgn}(\varepsilon_{s;\sigma}-\mu)\,e_{s'}}, \quad (251)$$

from which $\Sigma^{(1)}_{\sigma}(\varepsilon)$ follows according to $\Sigma^{(1)}_{\sigma}(\varepsilon)=\lim_{\eta\downarrow 0}\widetilde{\Sigma}^{(1)}_{\sigma}(\varepsilon\pm i\eta)$, $\varepsilon \gtrless \mu$ (*cf.* Eq. (65)). From the expression in Eq. (251), one straightforwardly infers

$$\widetilde{\Sigma}^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)\sim\Sigma^{\rm HF}(\boldsymbol{r},\boldsymbol{r}';[\varrho_{\sigma}])+\frac{\Sigma^{(1)}_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')}{z} +\frac{\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')}{z^2}+\frac{\Sigma^{(1)}_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')}{z^3},\;\; |z|\to\infty. \quad (252)$$

Here we deal with one more asymptotic term than in the case of the exact $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ (see Eq. (72) above); this will be helpful in identifying some characteristic features of $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ which this function has in common with $\widetilde{\Sigma}^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$. A comparison of the RHS of Eq. (252) with that of Eq. (72) (in combination with Eq. (62)) reveals that the leading term in the AS of $\Sigma^{(1)}_{\sigma}(\varepsilon)$ for $|\varepsilon|\to\infty$ coincides with that of the *exact* $\Sigma_{\sigma}(\varepsilon)$.

Employing the binomial series expansions of $\big(\varepsilon_{s;\sigma}+\mathrm{sgn}(\varepsilon_{s;\sigma}-\mu)e_{s'}\big)^m$, $m=0,1,2,\dots$, in the RHS of Eq. (251), after some algebraic manipulations, for the functions introduced in Eq. (252) we obtain

$$\Sigma^{(1)}_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')\equiv\frac{1}{2\hbar^2}G_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')W'_{\infty_1}(\boldsymbol{r},\boldsymbol{r}') \equiv\frac{1}{\hbar}\big\{\sum_{s',\sigma'}|w_{s';\sigma'}(\boldsymbol{r})|^2\big\}\,\delta(\boldsymbol{r}-\boldsymbol{r}'), \quad (253)$$

$$\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')\equiv\frac{1}{2\hbar^2}G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')W'_{\infty_1}(\boldsymbol{r},\boldsymbol{r}') +\frac{1}{2\hbar^2}G_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')W'_{\infty_2}(\boldsymbol{r},\boldsymbol{r}') -\frac{1}{\hbar}\varrho_{\sigma}(\boldsymbol{r}',\boldsymbol{r})W'_{\infty_2}(\boldsymbol{r},\boldsymbol{r}'), \quad (254)$$

$$\Sigma^{(1)}_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')\equiv\frac{1}{2\hbar^2}G_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')W'_{\infty_1}(\boldsymbol{r},\boldsymbol{r}') +\frac{1}{\hbar^2}G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')W'_{\infty_2}(\boldsymbol{r},\boldsymbol{r}') +\frac{1}{2\hbar^2}G_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')W'_{\infty_3}(\boldsymbol{r},\boldsymbol{r}') -\frac{2}{\hbar}\mathcal{D}_{\sigma}(\boldsymbol{r},\boldsymbol{r}')W'_{\infty_2}(\boldsymbol{r},\boldsymbol{r}'). \quad (255)$$

From these expressions, one readily observes that, in agreement with our earlier statement, whereas $\widetilde{W}'(z)$ is determined by W'_{∞_m}, $m=2,4,\dots$, the terms in the large-$|z|$ AS for $\widetilde{\Sigma}^{(1)}_{\sigma}(z)$ are determined by $\widetilde{W}'_{\infty_m}(z)$, $m=1,2,\dots$. This interesting aspect can be understood by realizing the fact that although the representation for $\widetilde{W}(z)$ in Eq. (249) similar to that for $\widetilde{G}_{\sigma}(z)$ in Eq. (27) is *exact*, *no* finite-order truncation of the sum on the RHS of Eq. (249) is capable of correctly reproducing $\widetilde{W}(z)$ in a neighbourhood of $z=0$; in other words, in evaluating the ε' integral on the RHS of Eq. (241), the summation over s corresponding to $W(\boldsymbol{r},\boldsymbol{r}';\varepsilon')$ (see Eqs. (242) and (249)) has to be carried out first (for otherwise one has to do with integrands that are non-integrably singular at $\varepsilon'=0$), thus resulting in an expression involving W'_{∞_m} for *all* m.

It can be shown that an approximation scheme that is capable of reproducing the exact W'_{∞_2} (see later) yields a $\widetilde{W}'(z)$ that satisfies the f-sum rule; however, unless such an approximation yield the exact W'_{∞_1}, already $\Sigma^{(1)}_{\sigma;\infty_1}$ ($\equiv\Sigma'^{(1)}_{\sigma;\infty_1}$) deviates from the expected $\Sigma^{(1)}_{\sigma;\infty_1}$ (Engel, *et al.* 1991). As we demonstrate below, the latter function itself deviates from that according to the exact theory, that is $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ as presented in Eq. (185) above. It follows that, in certain applications, an approximately-evaluated $\Sigma^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ may yield more accurate results than a $\Sigma^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ that is evaluated more accurately. This observation is clearly borne out by the calculations reported by Farid (1997a).

Before proceeding with the evaluation of the contributions on the RHSs of Eqs. (253) - (255) in terms of the GS correlation functions $\{\Gamma^{(m)}\}$, we indicate three noteworthy observations that are directly made from the expressions in Eqs. (252) and (253).

— Firstly, formally the leading term in the AS of $\widetilde{\Sigma}_{\sigma}^{(1)}(z)$, for $|z| \to \infty$, that is $\Sigma_{\sigma;\infty_0}^{(1)}$, coincides with that of the *exact* $\widetilde{\Sigma}_{\sigma}(z)$ (see Eq. (173) above); in practice, however, since the $\Sigma^{\rm HF}(\boldsymbol{r},\boldsymbol{r}';[\varrho_{\sigma}])$ on the RHS of Eq. (252) is *necessarily* evaluated in terms of a 'non-interacting', or Slater-Fock, density matrix $\varrho_{{\rm s};\sigma}(\boldsymbol{r},\boldsymbol{r}')$ (which, among others, in contrast with the interacting $\varrho_{\sigma}(\boldsymbol{r},\boldsymbol{r}')$ *is* idempotent; see Appendix C), this contribution deviates from the exact $\Sigma^{\rm HF}(\boldsymbol{r},\boldsymbol{r}';[\varrho_{\sigma}])$.

— Secondly, the next-to-leading asymptotic term pertaining to $\widetilde{\Sigma}_{\sigma}^{(1)}(\boldsymbol{r},\boldsymbol{r}';z)$, for $|z| \to \infty$, that is $\Sigma_{\sigma;\infty_1}^{(1)}$, is purely *local*, in evident contrast with the exact result presented in Eq. (185) above (see Eqs. (187) and (188)).

— Thirdly, the latter, purely local asymptotic contribution does *not* explicitly depend on the spin index σ, which amounts to a manifest shortcoming (see specifically the discussions in § V).

Below we evaluate the expressions for the various functions that feature on the RHSs of Eqs. (253) - (255), in terms of GS correlation functions $\{\Gamma^{(m)}\}$ (see Appendix B). In view of our extensive considerations in the earlier parts of this work (as well as in some related Appendices) in regard to *exact* functions $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, $m = 0,1,2$, below we shall *not* be exhaustive and thus mainly concentrate on some specific aspects of the indicated expressions.

A. Evaluation of $\Sigma_{\sigma;\infty_1}^{(1)}(\boldsymbol{r},\boldsymbol{r}')$

From the definitions in Eqs. (250), (245) and (246), making use of the completeness relation for $\big\{|\Psi_{N;s}\rangle\big\}$ in the Hilbert space of $(N_{\sigma}+N_{\bar{\sigma}})$-particle states, that is $I = \sum_s |\Psi_{N_{\sigma},N_{\bar{\sigma}};s}\rangle\langle\Psi_{N_{\sigma},N_{\bar{\sigma}};s}|$, and subsequently the normal ordering of the involved field operators, we obtain

$$W'_{\infty_1}(\boldsymbol{r},\boldsymbol{r}') = 2\int {\rm d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')n(\boldsymbol{r}'') -2\sum_{\sigma} v_H(\boldsymbol{r};[n_{\sigma}])v_H(\boldsymbol{r}';[n_{\sigma}]) + 2\mathcal{C}(\boldsymbol{r},\boldsymbol{r}'), \tag{256}$$

where $\mathcal{C}(\boldsymbol{r},\boldsymbol{r}')$ is defined in Eq. (B30) (see Appendix B). From Eqs. (253) and (256) we therefore have

$$\Sigma_{\sigma;\infty_1}^{(1)}(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{\hbar}\big[\mathcal{C}(\boldsymbol{r},\boldsymbol{r}) - \sum_{\sigma'} v_H^2(\boldsymbol{r};[n_{\sigma'}]) + \int {\rm d}^d r''\; v^2(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')\big]\delta(\boldsymbol{r}-\boldsymbol{r}'), \tag{257}$$

to be compared with $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (185) (see also Eqs. (187) and (188)). We point out that for systems in which $n_{\sigma}(\boldsymbol{r}) \equiv \frac{1}{2{\sf s}+1} n(\boldsymbol{r})$ holds for *all* σ (the 'paramagnetic' state of systems of spin-${\sf s}$ fermions), invoking the linearity of the Hartree potential in regard to its dependence on the number density, we have

$$\sum_{\sigma'} v_H(\boldsymbol{r};[n_{\sigma'}])v_H(\boldsymbol{r}';[n_{\sigma'}]) = \frac{1}{2{\sf s}+1}\, v_H(\boldsymbol{r};[n])v_H(\boldsymbol{r}';[n]).$$

This clearly brings out the most significant *quantitative* difference between $v_H(\boldsymbol{r};[n])v_H(\boldsymbol{r};[n])$ on the RHS of Eq. (185) and $\sum_{\sigma'} v_H(\boldsymbol{r};[n_{\sigma'}])v_H(\boldsymbol{r}';[n_{\sigma'}])$ on the RHS of Eq. (257).

Within the framework in which the N-particle GS wavefunction is approximated by a SSD (see Appendix C), one has (below, as elsewhere in this work, we indicate application of this approximation by either '$|_{\rm s}$' or a subscript 's', to be distinguished from 's')

$$\Sigma_{\sigma;\infty_1}^{(1)}(\boldsymbol{r},\boldsymbol{r}')\Big|_{\rm s} = \mathcal{A}'_{\rm s}(\boldsymbol{r},\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{258}$$

We present the expression for $\mathcal{A}'_{\rm s}(\boldsymbol{r},\boldsymbol{r}')$, the SSDA to $\mathcal{A}'(\boldsymbol{r},\boldsymbol{r}')$, defined in Eq. (F3), in Eq. (F74) (see also Eqs. (F66) and (F67)). The RHS of Eq. (258) coincides with the *local* part of the *exact* $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ with the N-particle GS similarly replaced by a SSD, that is (see Eq. (187) above)

$$\Sigma^{\rm l}_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')\big|_{\rm s} \equiv \Sigma_{\sigma;\infty_1}^{(1)}(\boldsymbol{r},\boldsymbol{r}')\Big|_{\rm s}. \tag{259}$$

In view of the fact that $\Sigma_{\sigma;\infty_1}^{(1)}(\boldsymbol{r},\boldsymbol{r}')$ is purely *local* and in view of Eq. (259), it is of interest to mention that, within the SSDA, for the *non-local* ('nl') part of the *exact* $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ one has

$$\Sigma^{\rm nl}_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')\big|_{\rm s} = -v^2(\boldsymbol{r}-\boldsymbol{r}')\varrho_{\sigma}(\boldsymbol{r}',\boldsymbol{r}) + \int {\rm d}^d r''\;\big[v(\boldsymbol{r}-\boldsymbol{r}')v(\boldsymbol{r}-\boldsymbol{r}'') + v(\boldsymbol{r}-\boldsymbol{r}')v(\boldsymbol{r}'-\boldsymbol{r}'') - v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\big]\varrho_{{\rm s};\sigma}(\boldsymbol{r}',\boldsymbol{r}'')\varrho_{{\rm s};\sigma}(\boldsymbol{r}'',\boldsymbol{r}). \tag{260}$$

The non-triviality of this result makes evident that indeed $\widetilde{\Sigma}_{\sigma}^{(1)}(\boldsymbol{r},\boldsymbol{r}';z)$ neglects a category of correlation effects already at order $1/z$. This is readily understood by considering the fact (see §§ III.E.1,3) that the *exact* $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ is, in its *explicit* dependence on v, a *quadratic* functional of v and thus must not be capable of being correctly described within the framework of a *first-order* perturbation theory. In general, and disregarding the possibility that, for arbitrary m, $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ can involve fundamentally unbounded contributions (see §§II.B and III), this function *explicitly* depends to *all* orders from the second (assuming $m \ge 1$) up to and including the $(m+1)$th order on v (see § II.B, the paragraph starting with '— Secondly, considering for the moment

…'; see also Eqs. (107) - (109) above), so that analogously $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ *cannot* be capable of being correctly described within the framework of a pth-order perturbation theory when $p \leq m$. In this connection we point out that the difference between the exact $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ and its counterpart within the framework of the SSDA lies in the *implicit* dependence of these functions on v, with the former depending to *all* orders on v.

Considering the intimate relationship between the set of $\Sigma_{\sigma;\infty_m}$, $m = 0, 1, \dots$, and the ε moments of the single-particle spectral function (see §§ III.B and III.E.6 as well as § III.I.2), one directly observes how SE operators evaluated at *finite* orders in the perturbation theory are fundamentally incapable of reproducing the *exact* single-particle excitation spectra. In this connection it is important to bear in mind how a change by ± 1 in the order of the perturbation series for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, can give rise to appearance or disappearance of contributions (which in specific contexts may or may not be significant) to the calculated SE; in the case considered above, the second-order contribution at issue turns out to be nothing less than the *entire* non-local contribution to $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ at order $1/z$ for $|z| \to \infty$.

B. Evaluation of $\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$

From Eq. (254) we observe that, with the exception of $W'_{\infty_2}(\boldsymbol{r},\boldsymbol{r}')$, in earlier Sections we have already determined all functions that contribute to the expression for $\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$.

From Eqs. (250), (245) and (246) we have

$$W'_{\infty_2}(\boldsymbol{r},\boldsymbol{r}') \equiv 2\sum_{s',\sigma'} e_{s'} w_{s',\sigma'}(\boldsymbol{r}) w^*_{s',\sigma'}(\boldsymbol{r}')$$
$$= 2\int \mathrm{d}^d r''_1 \mathrm{d}^d r''_2 \; v(\boldsymbol{r}-\boldsymbol{r}''_1) v(\boldsymbol{r}'-\boldsymbol{r}''_2) \Upsilon_1(\boldsymbol{r}''_1,\boldsymbol{r}''_2), \quad (261)$$

in which

$$\Upsilon_1(\boldsymbol{r}_1,\boldsymbol{r}_2) := \sum_{s',\sigma'} e_{s'} \rho_{s';\sigma'}(\boldsymbol{r}_1) \rho_{s';\sigma'}(\boldsymbol{r}_2)$$
$$= \sum_{\sigma'} \langle \Psi_{N;0}| \Big\{ \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}_1) \widehat{A}_{\sigma'}(\boldsymbol{r}_1) - \widehat{A}^\dagger_{\sigma'}(\boldsymbol{r}_1) \hat{\psi}_{\sigma'}(\boldsymbol{r}_1) \Big\} \times \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}_2) \hat{\psi}_{\sigma'}(\boldsymbol{r}_2) |\Psi_{N;0}\rangle, \quad (262)$$

where $\widehat{A}_\sigma(\boldsymbol{r})$ is defined in Eq. (158). Making use of the anticommutation relations in Eq. (29) and some algebra, we deduce

$$\Upsilon_1(\boldsymbol{r}_1,\boldsymbol{r}_2) = \lim_{\tilde{\boldsymbol{r}}_1 \to \boldsymbol{r}_1} \tau(\boldsymbol{r}_1) \Big\{ \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) \sum_{\sigma'} \varrho_{\sigma'}(\tilde{\boldsymbol{r}}_1,\boldsymbol{r}_1) - \delta(\tilde{\boldsymbol{r}}_1 - \boldsymbol{r}_2) \sum_{\sigma'} \varrho_{\sigma'}(\boldsymbol{r}_1,\boldsymbol{r}_2) \Big\}, \quad (263)$$

which upon substitution in Eq. (261) results in

$$W'_{\infty_2}(\boldsymbol{r},\boldsymbol{r}') = \frac{-\hbar^2}{m_e} \int \mathrm{d}^d r'' \; v(\boldsymbol{r}-\boldsymbol{r}'') \times \boldsymbol{\nabla}_{\boldsymbol{r}''} \cdot \big(n(\boldsymbol{r}'') \boldsymbol{\nabla}_{\boldsymbol{r}''} v(\boldsymbol{r}'-\boldsymbol{r}'') \big). \quad (264)$$

In obtaining this result, we have employed

$$\lim_{\tilde{\boldsymbol{r}} \to \boldsymbol{r}} \boldsymbol{\nabla}_{\boldsymbol{r}} \varrho_\sigma(\tilde{\boldsymbol{r}},\boldsymbol{r}) = \frac{1}{2} \boldsymbol{\nabla}_{\boldsymbol{r}} n_\sigma(\boldsymbol{r}), \quad (265)$$

which follows from the symmetry property $\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \equiv \varrho_\sigma(\boldsymbol{r},\boldsymbol{r}')$ (see Appendix B). We draw attention to the fact that, were $W'(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ evaluated in terms of the non-interacting state $|\Phi_{N;0}\rangle$ (to be contrasted with $|\Psi_{N;0}\rangle$ on the RHS of Eq. (245)), the total number density $n(\boldsymbol{r}'')$ on the RHS of Eq. (264) would have to be $n_{\rm s}(\boldsymbol{r}'')$ corresponding to $|\Phi_{N;0}\rangle$ (Engel and Farid 1993). For $|\Phi_{N;0}\rangle$ coinciding with the GS of the 'non-interacting' Hamiltonian due to Kohn and Sham (1965) within the framework of the GS density-functional theory, the corresponding $n_s(\boldsymbol{r}'')$ by construction is identical with $n(\boldsymbol{r})$ (for this to be possible, it is, however, required that $n(\boldsymbol{r})$ be so-called 'pure-state non-interacting v-representable'; for details see Dreizler and Gross 1990; see also Farid (1998)). Thus, for instance, the $W'^{\,\rm RPA}_{\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ corresponding to $W'^{\,\rm RPA}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ as evaluated in terms of the single-particle GF of the Kohn-Sham Hamiltonian associated with the GS of $\widehat{H}$, is *identical* with the *exact* $W'_{\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ (Farid 1999b); see footnote 7.

Making use of Eq. (168) which in conjunction with the closure relation for the Lehmann amplitudes in Eq. (30) yields

$$\sum_s^{>} f_{s;\sigma}(\boldsymbol{r}) f^*_{s;\sigma}(\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}') - \varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}), \quad (266)$$

with $\sum_s^{>}$ denoting a sum over all s corresponding to $\varepsilon_{s;\sigma} > \mu$ (see text following Eq. (168) above), from Eqs. (254), (162), (256), (30) and (264) we obtain

$$\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{\hbar} \Big\{ \int \mathrm{d}^d r'' \; v(\boldsymbol{r}-\boldsymbol{r}'') v(\boldsymbol{r}'-\boldsymbol{r}'') n(\boldsymbol{r}'') - \sum_{\sigma'} v_H(\boldsymbol{r};[n_{\sigma'}]) v_H(\boldsymbol{r}';[n_{\sigma'}]) + \mathcal{C}(\boldsymbol{r},\boldsymbol{r}') \Big\} \times \frac{1}{\hbar} G_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') + \frac{1}{\hbar} \big\{ \delta(\boldsymbol{r}-\boldsymbol{r}') - 2\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \big\} \times \frac{-\hbar^2}{2m_e} \int \mathrm{d}^d r'' \; v(\boldsymbol{r}-\boldsymbol{r}'') \boldsymbol{\nabla}_{\boldsymbol{r}''} \cdot \big(n(\boldsymbol{r}'') \boldsymbol{\nabla}_{\boldsymbol{r}''} v(\boldsymbol{r}'-\boldsymbol{r}'') \big). \quad (267)$$

We have *not* attempted to present the above expression in such a way as to make explicit the *local* and *non*-local contributions to $\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$. The expression in Eq. (267) is of interest to us, firstly, because a cursory comparison of it with its *exact* counterpart (see

Eqs. (185), (187) and (188) above) immediately reveals the extent to which $\Sigma_{\sigma;\infty_2}^{(1)}(\boldsymbol{r},\boldsymbol{r}')$ neglects interaction effects, [100] and secondly, because it exposes a contribution which in the case of $v \equiv v_c$ in $d=3$ is fundamentally unbounded and which is directly associated with an equally fundamentally unbounded contribution in the formal expression for $\Sigma_{\sigma;\infty_3}^{(1)}(\boldsymbol{r},\boldsymbol{r}')$ that we shall consider later. In all essential aspects, these unbounded contributions conform with our deductions on the basis of the expressions for the *exact* $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ corresponding to $m \le 2$ as regards the *complete* infinite series of unbounded contributions whose summation (see § III.H.2) accounts for a singular contribution to the finite-order AS for $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ decaying like $1/|z|^{3/2}$ as $|z|\to\infty$ (see Eqs. (210), (213) and (G11) - (G15)). Before entering into details, we mention that the required symmetry of $\Sigma_{\sigma;\infty_2}^{(1)}(\boldsymbol{r},\boldsymbol{r}')$ with respect to the exchange $\boldsymbol{r} \rightleftharpoons \boldsymbol{r}'$, which is *not* explicit in the term arising from the product of $\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$ with the last integral on the RHS of Eq. (267), is made explicit through applying the divergence theorem (or its generalizations in $d \neq 3$) which gives rise to the symmetric integrand $[\boldsymbol{\nabla}_{\boldsymbol{r}''} v(\boldsymbol{r}-\boldsymbol{r}'')]\cdot[\boldsymbol{\nabla}_{\boldsymbol{r}''} v(\boldsymbol{r}'-\boldsymbol{r}'')] n(\boldsymbol{r}'')$.

Now we consider the following expression whose LHS originates from the RHS of Eq. (267),

$$\frac{-\hbar^2}{2m_e}\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\boldsymbol{\nabla}_{\boldsymbol{r}''}\cdot\big(n(\boldsymbol{r}'')\boldsymbol{\nabla}_{\boldsymbol{r}''} v(\boldsymbol{r}'-\boldsymbol{r}'')\big)$$
$$\equiv \frac{-\hbar^2}{2m_e}\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')[\boldsymbol{\nabla}_{\boldsymbol{r}''} v(\boldsymbol{r}'-\boldsymbol{r}'')]\cdot[\boldsymbol{\nabla}_{\boldsymbol{r}''} n(\boldsymbol{r}'')]$$
$$+\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'') n(\boldsymbol{r}'')\,\big(\tau(\boldsymbol{r}'') v(\boldsymbol{r}'-\boldsymbol{r}'')\big). \qquad (268)$$

When multiplied by $\frac{1}{\hbar}\delta(\boldsymbol{r}-\boldsymbol{r}')$, the last term on the RHS of Eq. (268) is seen to be identical with a term in the expression for the *exact* $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (199) (see $\mathcal{I}_3$ as defined in Eq. (202) above). The identity of the two terms implies that in the expression for $\Sigma_{\sigma;\infty_3}^{(1)}(\boldsymbol{r},\boldsymbol{r}')$, to be discussed in the following Section, we have to find a term identical with the term that we infer in Appendix G from the general structure of the *exact* $\{\Sigma_{\sigma;\infty_m}\|m\le 2\}$. This indeed turns out to be the case.

[100] Note for instance that the approximation in Eq. (267) does *not* involve the contribution $-v^3(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$, which is explicit in the expression for the *exact* $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ on the RHS of Eq. (199) (see also Eq. (212)); as we discuss in Appendix H, this contribution, which is *non*-integrable in the case of $v\equiv v_c$ in $d=3$, following an infinite-order summation of related non-integrable functions in $\{\Sigma_{\sigma;\infty_m}\|m\ge 2\}$, gives rise to a *singular* contribution to the large-$|z|$ AS pertaining to the momentum representation of $\widetilde{\Sigma}_\sigma(z)$.

C. Evaluation of $\Sigma_{\sigma;\infty_3}^{(1)}(\boldsymbol{r},\boldsymbol{r}')$

From Eqs. (250), (245) and (246), making repeated use of the anticommutation relations in Eq. (29), we obtain

$$W'_{\infty_3}(\boldsymbol{r},\boldsymbol{r}') \equiv 2\sum_{s',\sigma'} e_{s'}^2\, w_{s',\sigma'}(\boldsymbol{r}) w_{s',\sigma'}^*(\boldsymbol{r}')$$
$$= 2\int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}'-\boldsymbol{r}_2'')\Upsilon_2(\boldsymbol{r}_1'',\boldsymbol{r}_2''), \qquad (269)$$

in which

$$\Upsilon_2(\boldsymbol{r}_1,\boldsymbol{r}_2) := \sum_{s',\sigma'} e_{s'}^2\,\rho_{s';\sigma'}(\boldsymbol{r}_1)\rho_{s';\sigma'}(\boldsymbol{r}_2)$$
$$= \sum_{\sigma'}\langle\Psi_{N;0}|\Big\{\widehat{B}_{\sigma'}(\boldsymbol{r}_1)+\widehat{B}_{\sigma'}^\dagger(\boldsymbol{r}_1)-2\widehat{A}_{\sigma'}^\dagger(\boldsymbol{r}_1)\widehat{A}_{\sigma'}(\boldsymbol{r}_1)\Big\}$$
$$\times\hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r}_2)\hat{\psi}_{\sigma'}(\boldsymbol{r}_2)|\Psi_{N;0}\rangle, \qquad (270)$$

where $\hat{A}_\sigma(\boldsymbol{r})$ is defined in Eq. (158) and

$$\widehat{B}_\sigma(\boldsymbol{r}) := \hat{\psi}_\sigma^\dagger(\boldsymbol{r})\big[\widehat{A}_\sigma(\boldsymbol{r}),\widehat{H}\big]_-$$
$$= \hat{\psi}_\sigma^\dagger(\boldsymbol{r})\widehat{A}_\sigma(\boldsymbol{r})\widehat{H} + \widehat{A}_\sigma^\dagger(\boldsymbol{r})\widehat{A}_\sigma(\boldsymbol{r}) - \widehat{H}\hat{\psi}_\sigma^\dagger(\boldsymbol{r})\widehat{A}_\sigma(\boldsymbol{r}). \quad (271)$$

After some algebra, we deduce

$$\Upsilon_2(\boldsymbol{r}_1,\boldsymbol{r}_2) = \sum_{\sigma'}\varrho_{\sigma'}(\boldsymbol{r}_1,\boldsymbol{r}_2)\tau(\boldsymbol{r}_1)\tau(\boldsymbol{r}_2)\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)$$
$$-\big[\tau(\boldsymbol{r}_2)\sum_{\sigma'}\varrho_{\sigma'}(\boldsymbol{r}_1,\boldsymbol{r}_2)\big]\tau(\boldsymbol{r}_1)\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)$$
$$-\big[\tau(\boldsymbol{r}_1)\sum_{\sigma'}\varrho_{\sigma'}(\boldsymbol{r}_1,\boldsymbol{r}_2)\big]\tau(\boldsymbol{r}_2)\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)$$
$$+\big[\tau(\boldsymbol{r}_1)\tau(\boldsymbol{r}_2)\sum_{\sigma'}\varrho_{\sigma'}(\boldsymbol{r}_1,\boldsymbol{r}_2)\big]\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)$$
$$+2\lim_{\substack{\tilde{\boldsymbol{r}}_1\to\boldsymbol{r}_1\\ \tilde{\boldsymbol{r}}_2\to\boldsymbol{r}_2}}\tau(\boldsymbol{r}_1)\tau(\boldsymbol{r}_2)$$
$$\times\sum_{\sigma'}\Big\{\Gamma^{(2)}(\tilde{\boldsymbol{r}}_1\sigma',\boldsymbol{r}_2\sigma';\boldsymbol{r}_1\sigma',\tilde{\boldsymbol{r}}_2\sigma')$$
$$-\Gamma^{(2)}(\tilde{\boldsymbol{r}}_1\sigma',\tilde{\boldsymbol{r}}_2\sigma';\boldsymbol{r}_1\sigma',\boldsymbol{r}_2\sigma')\Big\}, \qquad (272)$$

which on substitution in the expression on the RHS of Eq. (269) results in

$$W'_{\infty_3}(\boldsymbol{r},\boldsymbol{r}') = 2\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')$$
$$\times\lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''}\tau^2(\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\sum_{\sigma'}\varrho_{\sigma'}(\tilde{\boldsymbol{r}}'',\boldsymbol{r}'')$$
$$-2\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''}\tau(\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')$$
$$\times\big[\tau(\boldsymbol{r}'')\sum_{\sigma'}\varrho_{\sigma'}(\tilde{\boldsymbol{r}}'',\boldsymbol{r}'')\big]$$
$$-2\int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')\lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''}\tau(\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'')$$

$$\times\big[\tau(\boldsymbol{r}'')\sum_{\sigma'}\varrho_{\sigma'}(\boldsymbol{r}'',\tilde{\boldsymbol{r}}'')\big]$$
$$+2\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')$$
$$\times \lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''}\tau(\boldsymbol{r}'')\tau(\tilde{\boldsymbol{r}}'')\sum_{\sigma'}\varrho_{\sigma'}(\boldsymbol{r}'',\tilde{\boldsymbol{r}}'')$$
$$+4\int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}'-\boldsymbol{r}_2'')$$
$$\times \lim_{\substack{\tilde{\boldsymbol{r}}_1''\to\boldsymbol{r}_1''\\ \tilde{\boldsymbol{r}}_2''\to\boldsymbol{r}_2''}}\tau(\boldsymbol{r}_1'')\tau(\boldsymbol{r}_2'')$$
$$\times\sum_{\sigma'}\Big\{\Gamma^{(2)}(\tilde{\boldsymbol{r}}_1''\sigma',\boldsymbol{r}_2''\sigma';\boldsymbol{r}_1''\sigma',\tilde{\boldsymbol{r}}_2''\sigma')$$
$$-\Gamma^{(2)}(\tilde{\boldsymbol{r}}_1''\sigma',\tilde{\boldsymbol{r}}_2''\sigma';\boldsymbol{r}_1''\sigma',\boldsymbol{r}_2''\sigma')\Big\}. \qquad (273)$$

Making use of the general result

$$\tau^2 fg = [\tau^2 f]g + f[\tau^2 g] + \dots, \qquad (274)$$

we have, for the first integral on the RHS of Eq. (273),

$$\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''}\tau^2(\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\times\sum_{\sigma'}\varrho_{\sigma'}(\tilde{\boldsymbol{r}}'',\boldsymbol{r}'')$$
$$=\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')\big(\tau^2(\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\big)+\dots, \qquad (275)$$

which gives rise to the following result for the first term on the RHS of Eq. (255) concerning $\Sigma^{(1)}_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')$ (see Eq. (30) above):

$$\frac{1}{2\hbar^2}G_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')W'_{\infty_3}(\boldsymbol{r},\boldsymbol{r}')=\frac{1}{\hbar}\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')\times\big(\tau^2(\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'')\big)\,\delta(\boldsymbol{r}-\boldsymbol{r}')+\dots. \qquad (276)$$

The (local) contribution which we have explicitly presented on the RHS of Eq. (276), *exactly* coincides with what is inferred from the expressions for the *exact* $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, with $m=1,2$, in Appendix G. However, since $\Sigma^{(1)}_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ does *not* contain a *non*-local contribution, *nor* does the *non*-local contribution pertaining to $\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ involve a term similar to that on the RHS of Eq. (203) (see also Eq. (207) above), from our above considerations it follows that, in regard to $\widetilde{\Sigma}^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$, the equivalent of $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$, defined in Eq. (G1), is the following:

$$\widetilde{\mathsf{T}}^{(1)}(\boldsymbol{r};z):=\frac{1}{z}\sum_{m=1}^{\infty}\int \mathrm{d}^3 r''\; v_c(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')\times\big[\frac{1}{z^m}\tau^m(\boldsymbol{r}'')v_c(\boldsymbol{r}-\boldsymbol{r}'')\big]$$
$$=\frac{1}{z^2}\int \mathrm{d}^3 r''\; v_c(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')\times\tau(\boldsymbol{r}'')\big(1-\frac{1}{z}\tau(\boldsymbol{r}'')\big)^{-1}v_c(\boldsymbol{r}-\boldsymbol{r}''), \qquad (277)$$

which in contrast with $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$ does *not* explicitly depend on σ. All the results concerning $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$, determined in Appendix G, are directly applicable to $\widetilde{\mathsf{T}}^{(1)}(\boldsymbol{r};z)$, with the sole requirement that $[n_{\bar{\sigma}}(\boldsymbol{r})-n_{\sigma}(\boldsymbol{r})]$ in the expressions associated with $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$ be replaced by $n(\boldsymbol{r})$. The considerable significance of $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$ in the case $v\equiv v_c$ in $d=3$ to the behaviour of $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ at large $|z|$ on the one hand (see § III.H.2), and the significant difference between $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$ and $\widetilde{\mathsf{T}}^{(1)}(\boldsymbol{r};z)$ on the other hand, unequivocally show a fundamental shortcoming of $\widetilde{\Sigma}^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ (see § IV). For later reference, in analogy with $\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})$ in Eq. (209) we define

$$\mathcal{T}^{(1)}(\boldsymbol{r}):=\int \mathrm{d}^3 r''\; v_c(\boldsymbol{r}-\boldsymbol{r}'')\,n(\boldsymbol{r}'')\times\big(\tau(\boldsymbol{r}'')v_c(\boldsymbol{r}-\boldsymbol{r}'')\big). \qquad (278)$$

Finally, because $G_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')\propto\delta(\boldsymbol{r}-\boldsymbol{r}')$ (see Eq. (30) above) and in view of Eq. (255), the contributions to $\Sigma^{(1)}_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')$ as arising from the second and third integrals on the RHS of Eq. (273), are for $v\equiv v_c$ in $d=3$ identical and fundamentally unbounded; these contributions are *partly* cancelled by the contribution from the first term on the RHS of Eq. (273), associated with a term on the RHS of Eq. (274) whose explicit form we have not presented. The existence of such unbounded contributions to $\Sigma^{(1)}_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')$ which are *not* related to any unbounded counterparts in the expression for $\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$, implies that (see § II.B) the $1/z^2$ term in the large-$|z|$ AS for $\widetilde{\Sigma}^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ is followed by a term, or terms, more dominant than $1/z^3$.

D. Correcting $\Sigma^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)\equiv\Sigma'^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)+\hbar^{-1}v_H(\boldsymbol{r};[n])\,\delta(\boldsymbol{r}-\boldsymbol{r}')$; a workable scheme

The considerations in the above three Sections, A, B and C have exposed the shortcomings of $\Sigma^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ as reflected in the behaviour of this function for 'large' values of $|\varepsilon|$. In view of our discussions in § III.B, it is evident that the deviation of $\Sigma^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ from its exact counterpart $\Sigma_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (see Eq. (240)) in the regime of large $|\varepsilon|$ implies deviation of the ε moments integrals of the associated single-particle spectral function from those of the exact $A_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$. With our knowledge of the first few terms in the large-$|\varepsilon|$ AS of the *exact* $\Sigma_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (as well as those of $\Sigma^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$), fully expressed in terms of GS correlation functions, we are in a position to correct for the above-mentioned shortcomings of $\Sigma^{(1)}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, while retaining a function applicable for *all* values of ε. For simplicity of notation, in the following we employ

$\mathsf{f}(\varepsilon)$ as denoting [101] $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ for which we consider the following large-$|\varepsilon|$ AS

$$\mathsf{f}(\varepsilon) \sim \mathsf{f}_0 + \frac{\mathsf{f}_1' + i\,\mathsf{f}_1''}{\varepsilon} + \frac{[\Theta(\mu-\varepsilon) - i\Theta(\varepsilon-\mu)]\,\mathsf{f}_{3/2}}{|\varepsilon|^{3/2}} + \frac{\ln|\varepsilon/\varepsilon_0|\,\mathsf{f}_{\rm ln}}{\varepsilon^2} + \frac{\mathsf{f}_2' + i\,[\mathsf{f}_2'' - \pi\Theta(\varepsilon-\mu)\,\mathsf{f}_{\rm ln}]}{\varepsilon^2}, \quad |\varepsilon|\to\infty, \tag{279}$$

where the coefficient functions f_0, f_1', f_1'', etc., are real valued (see Appendix B). In writing the expression in Eq. (279), we have assumed $\mathsf{f}_1 \equiv \mathsf{f}_1' + i\,\mathsf{f}_1''$ to be well defined so that, in cases where $v \equiv v_c$, it is required that $d = 3$ (see footnote 12 and § 1.a in Appendix F). Further, in the cases corresponding to bounded and short-range interaction functions v, we have $\mathsf{f}_{3/2} \equiv \mathsf{f}_{\rm ln} \equiv 0$. With reference to our considerations in § III.E.2 (see in particular Eq. (112); see also Eq. (229)), one readily identifies f_0 with $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')$, f_1' with $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ and f_2' with $\Sigma^{\rm r}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}') + \Sigma^{\rm s_b}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$; the imaginary parts f_1'' and f_2'' are the coefficients of $1/\varepsilon$ and $1/\varepsilon^2$ on the RHS of Eq. (227) (in identifying f_1'' and f_2'' with the latter coefficients, account has to be taken of the provisions indicated in the paragraphs subsequent to Eq. (227)); we point out, however, that, for the sake of simplicity of presentation, here we have exceptionally deviated from our general convention (see footnote 31 and text following Eq. (111) above) and incorporated $\hbar^{-1}\mathsf{M}^{\rm r}_{\infty_2}(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}')$, which is a component part of $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'\|z)$ (see Eqs. (213) and (F159)), into f_2'. Further, $\mathsf{f}_{3/2}$ and $\mathsf{f}_{\rm ln}$ directly *correspond to* $\hbar^{-1}\widetilde{\mathsf{T}}^{\rm s}_{\sigma,\bar\sigma;\infty_2}(\boldsymbol{r}\|z)\,\delta(\boldsymbol{r}-\boldsymbol{r}')$ (see Eqs. (G15) and (G17)) and $\hbar^{-1}\widetilde{\mathsf{M}}^{\rm s}_{\infty_2}(\boldsymbol{r}\|z)\,\delta(\boldsymbol{r}-\boldsymbol{r}')$ (see Eqs. (213) and (F160)) respectively; since we explicitly account for the ε-dependent parts of the latter functions in the expression on the RHS of Eq. (279), these parts are left out of $\mathsf{f}_{3/2}$ and $\mathsf{f}_{\rm ln}$.

It is interesting to note that for $v \equiv v_c$ and $d = 3$, $\mathsf{f}_{3/2}$ is *positive* for $n_{\bar\sigma}(\boldsymbol{r}) > n_\sigma(\boldsymbol{r})$, *zero* for $n_{\bar\sigma}(\boldsymbol{r}) = n_\sigma(\boldsymbol{r})$, and *negative* for $n_{\bar\sigma}(\boldsymbol{r}) < n_\sigma(\boldsymbol{r})$ (see Eqs. (G15), and (G17)), and further that $\mathsf{f}_{\rm ln}$ is *strictly positive* (see Eq. (F160)). Considering the fact that stability of the GS demands $\mathrm{Im}[\mathcal{E}_{\varsigma;\sigma}(\varepsilon)] \lesseqgtr 0$ for $\varepsilon \gtrless \mu$, $\forall\varsigma,\sigma$ (see § III.D, and in particular Eqs. (84) and (85)), the expression on the RHS of Eq. (279) is seen to expose a crucial balance that should exist between various imaginary contributions in the large-$|\varepsilon|$ AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ in order for an assumed (normal) GS, in terms of which these contributions are calculated, to be the true and stable GS of the system under consideration. In this light, one specifically clearly observes the significance of the interaction potentials $v(\boldsymbol{r}-\boldsymbol{r}')$ that for $\|\boldsymbol{r}-\boldsymbol{r}'\| \to 0$ behave like the Coulomb potential in $d = 3$ in bringing about particular GSs that otherwise would not be feasible; in this connection, recall that, for bounded interaction potentials, $\mathsf{f}_{3/2}$ is identically vanishing.

We are now in a position to introduce the scheme to which we have referred above; this scheme almost effortlessly removes the shortcomings of $\Sigma^{(1)}_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ as discussed in §§ IV.A, B, C. To this end, we consider an expression for the large-$|\varepsilon|$ AS of $\Sigma^{(1)}_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ which *functionally* is identical with that in Eq. (279), with $\mathsf{f}(\varepsilon)$, f_0, f_1', f_1'', $\mathsf{f}_{3/2}$, ... herein replaced by $\mathsf{f}^{(1)}(\varepsilon)$, $\mathsf{f}_0^{(1)}$, $\mathsf{f}_1'^{(1)}$, $\mathsf{f}_1''^{(1)}$, $\mathsf{f}_{3/2}^{(1)}$, ... respectively. Consider now the functions $\Phi_\alpha(\varepsilon,\mu;\Delta)$, $\alpha = 0, 1, 3/2, 2$, defined as follows:

$$\begin{aligned}
\Phi_0(\varepsilon,\mu;\Delta) &:= \frac{\varepsilon^4-\mu^4}{\varepsilon^4+\Delta^4} \sim 1 - \frac{\mu^4+\Delta^2}{\varepsilon^4} \quad \text{for} \quad |\varepsilon|\to\infty,\\
\Phi_1(\varepsilon,\mu;\Delta) &:= \frac{\varepsilon^5-\mu^5}{\varepsilon^6+\Delta^6} \sim \frac{1}{\varepsilon} - \frac{\mu^5}{\varepsilon^6} \quad \text{for} \quad |\varepsilon|\to\infty,\\
\Phi_{3/2}(\varepsilon,\mu;\Delta) &:= \frac{\varepsilon^6-\mu^6}{|\varepsilon|^{15/2}+\Delta^{15/2}} \sim \frac{1}{|\varepsilon|^{3/2}} - \frac{\mu^6}{|\varepsilon|^{15/2}} \quad \text{for} \quad |\varepsilon|\to\infty,\\
\Phi_2(\varepsilon,\mu;\Delta) &:= \frac{\varepsilon^6-\mu^6}{\varepsilon^8+\Delta^8} \sim \frac{1}{\varepsilon^2} - \frac{\mu^6}{\varepsilon^8} \quad \text{for} \quad |\varepsilon|\to\infty.
\end{aligned} \tag{280}$$

The characteristic aspects of these functions are that for $\varepsilon \to \mu$ they *smoothly* approach zero [102] and for $|\varepsilon| \to \infty$, not only are their leading-order terms 1, $1/\varepsilon$, $1/|\varepsilon|^{3/2}$ and $1/\varepsilon^2$ respectively (*cf.* Eq. (279)), but also their next-to leading-order terms *all* decay *more rapidly* than $1/\varepsilon^2$.

Let now $\mathsf{f}^{(1)}_{\rm m}(\varepsilon)$ denote the *modified* SE, deduced from the first-order SE $\mathsf{f}^{(1)}(\varepsilon)$, which we define as follows:

$$\begin{aligned}
\mathsf{f}^{(1)}_{\rm m}(\varepsilon) := {}&\mathsf{f}^{(1)}(\varepsilon) + \big[\mathsf{f}_0 - \mathsf{f}_0^{(1)}\big]\,\Phi_0(\varepsilon,\mu;\Delta_0)\\
&+ \big[\mathsf{f}_1' + i\mathsf{f}_1'' - \mathsf{f}_1'^{(1)} - i\mathsf{f}_1''^{(1)}\big]\,\Phi_1(\varepsilon,\mu;\Delta_1)\\
&+ \big[\Theta(\mu-\varepsilon) - i\Theta(\varepsilon-\mu)\big]\big[\mathsf{f}_{3/2} - \mathsf{f}_{3/2}^{(1)}\big]\,\Phi_{3/2}(\varepsilon,\mu;\Delta_{3/2})
\end{aligned}$$

[101] Owing to $\Sigma^{\rm s}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$, analogous considerations as below but concerning $\overline{\overline{\Sigma}}_\sigma(\boldsymbol{q},\boldsymbol{q}';\varepsilon)$, the momentum representation of $\Sigma_\sigma(\varepsilon)$, require some non-essential alteration of the following in the case where, for example, $v \equiv v_c$ and $d = 3$; see footnote 72. Insofar as homogeneous systems with uniform and isotropic GSs are concerned, the counterparts of the expression in Eq. (279) for the diagonal elements of the SE operator in the momentum representation are those in Eqs. (128) and (129) (by symmetry, the off-diagonal elements are identically vanishing).

[102] Specifically, they are continuously differentiable functions of ε in a neighbourhood of $\varepsilon = \mu$ so that, for the cases where the GS of the system under consideration is metallic, the modified SE, to be introduced in Eq. (281) below, is *not* by construction made to correspond to a non-Fermi-liquid metallic state (Farid 1999c); see Appendix A, the paragraph including Eq. (A61).

$$+\Big\{ \ln\left|\frac{\varepsilon-\mu}{\varepsilon_0}\right| \, \big[\mathsf{f}_{\rm ln} - \mathsf{f}_{\rm ln}^{(1)}\big] + \mathsf{f}_2' + i[\mathsf{f}_2'' - \pi\Theta(\varepsilon-\mu)\,\mathsf{f}_{\rm ln}] \\ -\mathsf{f}_2'^{(1)} - i[\mathsf{f}_2''^{(1)} - \pi\Theta(\varepsilon-\mu)\,\mathsf{f}_{\rm ln}^{(1)}]\Big\}\,\Phi_2(\varepsilon,\mu;\Delta_2), \tag{281}$$

where Δ_0, Δ_1, $\Delta_{3/2}$ and Δ_2 are finite constants (about which more later) and μ stands for the 'chemical potential' associated with $\mathsf{f}^{(1)}(\varepsilon)$, that is $\Sigma_\sigma^{(1)}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (see Eqs. (22) and (23) above). Assuming the latter function to have been evaluated in terms of the *exact* $G_\sigma(\varepsilon)$, from the expression on the RHS of Eq. (251) it can be readily deduced that the μ associated with $\mathsf{f}^{(1)}(\varepsilon)$ coincides with that associated with the *exact* $\mathsf{f}(\varepsilon)$. We should emphasize that for *non-metallic* GSs, where $\mu_{N;\sigma}^{+} - \mu_{N;\sigma}^{-}$ (see Eqs. (22) and (23) above) is finite, the statement with regard to the equality of the two 'chemical potentials', associated with $\mathsf{f}(\varepsilon)$ and $\mathsf{f}^{(1)}(\varepsilon)$, is rather meaningless, as for such GSs μ is *not* uniquely defined (the absolute temperature is assumed to be zero in our considerations); however, for metallic GSs, for which $\mu_{N;\sigma}^{+}-\mu_{N;\sigma}^{-} \sim 1/N^{\alpha}$, with $\alpha > 0$ (see footnote 60), the above statement concerning the two μ values is both meaningful and non-trivial. We note in passing, that the μ associated with the $\mathsf{f}^{(1)}(\varepsilon) \equiv \Sigma_\sigma^{(1)}(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (pertaining to a metallic GS; see above) evaluated in terms of the single-particle GF $G_{0;\sigma}(\varepsilon)$ pertaining to the *exact* 'non-interacting' Kohn-Sham (Kohn and Sham 1965) Hamiltonian associated with the GS of $\widehat{H}$ (Farid 1997a,b) equally coincides with the *exact* μ. For completeness, our considerations in Appendix A (§ 2 herein) indicate a way out also *explicitly* to correct the behaviour of $\mathsf{f}^{(1)}(\varepsilon)$ for ε close to μ (note that, there are some *implicit* 'corrections' to the behaviour of $\mathsf{f}^{(1)}(\varepsilon)$ for $\varepsilon \to \mu$, brought about by the global conditions to be satisfied by $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$, enforced through the choice of the parameters Δ_0, Δ_1, $\dots$ in Eq. (281); see later).

With reference to the appearance of $\ln|(\varepsilon-\mu)/\varepsilon_0|$ on the RHS of Eq. (281), to be contrasted with $\ln|\varepsilon/\varepsilon_0|$ on the RHS of Eq. (279), we point out that, because

$$\ln\left|\frac{\varepsilon-\mu}{\varepsilon_0}\right| \sim \ln\left|\frac{\varepsilon}{\varepsilon_0}\right| - \frac{\mu}{\varepsilon} \quad \text{for} \quad |\varepsilon| \to \infty,$$

the deviation of $\ln|(\varepsilon-\mu)/\varepsilon_0|$ from $\ln|\varepsilon/\varepsilon_0|$ gives rise to a contribution to the RHS of Eq. (281) that for $|\varepsilon| \to \infty$ decays like $1/\varepsilon^3$. This is by one power of $1/\varepsilon$ less significant than the least significant term on the RHS of Eq. (279) above. From this and in view of the large-$|\varepsilon|$ asymptotic results on the RHSs of the expressions in Eq. (280), it follows that for $|\varepsilon| \to \infty$, $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ by construction exactly reproduces the asymptotic expression corresponding to the *exact* $\mathsf{f}(\varepsilon)$ as presented in Eq. (279). In this connection, it is important to realize that taking account of *any* number of correction terms (and thus neglecting the remaining terms) on the RHS of Eq. (281) amounts to an improvement with respect to $\mathsf{f}^{(1)}(\varepsilon)$.

Concerning Δ_0, Δ_1, $\dots$ in the expression for $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ on the RHS of Eq. (281), these free parameters do *not* need to be all different and thus may in principle be identified with one parameter, Δ (see, however, later where we elaborate on the conditions to be satisfied by $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ which signify the importance of sufficient flexibility in the expression for $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ and thus of Δ_0, Δ_1, $\dots$). Similarly, one can consider an alternative expression for $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ where $[\mathsf{f}_0 - \mathsf{f}_0^{(1)}]\Phi_0(\varepsilon,\mu;\Delta_0)$, etc., is replaced by $\mathsf{f}_0\Phi_0(\varepsilon,\mu;\Delta_0') - \mathsf{f}_0^{(1)}\Phi_0(\varepsilon,\mu;\Delta_0'')$, etc., thus taking into account the possibility that $\mathsf{f}(\varepsilon)$, which $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ is supposed reliably to approximate, may differently approach its large-$|\varepsilon|$ asymptotic behaviour than $\mathsf{f}^{(1)}(\varepsilon)$. Further, although $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ depends on Δ_0, Δ_1, $\dots$ so long as these are identified with *finite* values, $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ exactly reproduces the RHS of Eq. (279) for sufficiently large values of $|\varepsilon|$. In spite of this, the following aspects have to be carefully considered in choosing the values for Δ_0, Δ_1, $\dots$.

— Firstly, as can be obtained from Eqs. (39) and (24),

$$A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon) = \hbar \sum_s f_{s;\sigma}(\boldsymbol{r}) f_{s;\sigma}^{*}(\boldsymbol{r}')\,\delta(\varepsilon - \varepsilon_{s;\sigma}), \tag{282}$$

from which one deduces not only that $A_\sigma(\boldsymbol{r},\boldsymbol{r};\varepsilon) \ge 0$, $\forall\varepsilon$, but also that $A_\sigma(\varepsilon)$, of which $A_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ is the coordinate representation, is a positive semi-definite operator for *all* ε. This essential property must be preserved.

— Secondly, by the requirement of conservation of particles of spin index σ, $\forall\sigma$, it is necessary that the single-particle spectral functions associated with the modified SEs, corresponding to all σ, satisfy the following equation

$$\frac{1}{\hbar}\int_{-\infty}^{\mu} {\rm d}\varepsilon \int {\rm d}^d r\; A_\sigma(\boldsymbol{r},\boldsymbol{r};\varepsilon) = N_\sigma, \;\; \forall\sigma, \tag{283}$$

where $\{N_\sigma\}$ is common to both the interacting and non-interaction GSs (see the paragraph containing Eqs. (54) and (55) above).

— Thirdly, too small values for Δ_0, Δ_1, $\dots$ gives rise to a relatively rapid variation of $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ for ε departing from μ, while too large values for these parameters entail that, for a relatively wide range of ε values away from $\varepsilon = \mu$, the behaviour of $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ is unduly dominated by that of $\mathsf{f}^{(1)}(\varepsilon)$. In view of the considerations in § III.E, it is natural to expect that for any interacting system there exists an energy, similar to e_0 defined in Eq. (103), with respect to which $|\varepsilon|$ can be considered as being 'small' or 'large' (for the specific system dealt with in § III.E, $|\varepsilon/e_0|$ is shown to be 'large' provided it is larger than $\max(1, r_s)$) and which sets the scale over which a change in ε produces a comparable change in $\hbar\mathsf{f}(\varepsilon)$. In this light we expect the parameters Δ_0, Δ_1, $\dots$ to be all on the order of the latter energy scale. Since $\mathsf{f}^{(1)}(\varepsilon)$ can be relatively easily calculated within the framework of the SSDA, one may deduce very good 'estimates' (see later) for Δ_0, Δ_1, $\dots$ by means of fitting

$$\begin{aligned}&\mathsf{f}_0^{(1)}\Phi_0(\varepsilon,\mu;\Delta_0)+\big[\mathsf{f}_1'^{(1)}+i\mathsf{f}_1''^{(1)}\big]\,\Phi_1(\varepsilon,\mu;\Delta_1)\\&\quad+\big[\Theta(\mu-\varepsilon)-i\Theta(\varepsilon-\mu)\big]\mathsf{f}_{3/2}^{(1)}\,\Phi_{3/2}(\varepsilon,\mu;\Delta_{3/2})\\&\quad+\Big\{\ln\Big\vert\frac{\varepsilon-\mu}{\varepsilon_0}\Big\vert\;\mathsf{f}_{\rm ln}^{(1)}+\mathsf{f}_2'^{(1)}\\&\qquad+i[\mathsf{f}_2''^{(1)}-\pi\Theta(\varepsilon-\mu)\,\mathsf{f}_{\rm ln}^{(1)}]\Big\}\,\Phi_2(\varepsilon,\mu;\Delta_2)\end{aligned}$$

to the directly calculated $\mathsf{f}^{(1)}(\varepsilon)$ at 'large' values of $|\varepsilon|$, taking into account the requirements indicated above, in particular those implied by Eq. (283). We note in passing that in practice it will be more convenient to obtain (at least) some of the coefficients $\mathsf{f}_0^{(1)}$, $\mathsf{f}_1'^{(1)}$, $\mathsf{f}_1''^{(1)}$, ... from the directly calculated $\mathsf{f}^{(1)}(\varepsilon)$ (by means of some appropriate fitting procedure), than to determine these through evaluation of the pertinent expressions presented in §§ IV.A, B, C. Consequently, direct calculation of $\mathsf{f}^{(1)}(\varepsilon)$ at 'large' values of $|\varepsilon|$ not only helps estimate the appropriate values for Δ_0, Δ_1, ... but also facilitates calculation of the sought-after coefficients $\mathsf{f}_0^{(1)}$, $\mathsf{f}_1'^{(1)}$, $\mathsf{f}_1''^{(1)}$, ...

— Fourthly, attention should be paid to the fact that since $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)-\mathsf{f}^{(1)}(\varepsilon)$ is *not* directly associated with a set of SE diagrams, $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ and the associated GF should *not* in general identically satisfy the Luttinger-Ward (1960) identity presented in Eq. (A68) (see the paragraph containing the indicated identity in Appendix A), so that this identity may be utilized as a subsidiary condition (complimentary to the non-negativity condition for $A_\sigma(\varepsilon)$ and those in Eq. (283) above) to be fulfilled in determining the parameters Δ_0, Δ_1, ...

We point out that, since determination of f_1'' and f_2'' requires the knowledge of the real part of the *exact* SE for $\varepsilon\in(-\infty,\infty)$ (see Eq. (227) above), in practice it is necessary first to consider $\mathrm{Re}[\mathsf{f}_{\rm m}^{(1)}(\varepsilon)]$ (whose expression does *not* involve, amongst others, f_1'' and f_2'') and subsequent to choosing some appropriate values for the parameters Δ_0, Δ_1, ..., determine $\mathrm{Im}[\mathsf{f}_{\rm m}^{(1)}(\varepsilon)]$ from the Kramers-Krönig relation in Eqs. (217) and (218). We should emphasize that, since all the above conditions concern $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$, rather that $\mathrm{Re}[\mathsf{f}_{\rm m}^{(1)}(\varepsilon)]$ and $\mathrm{Im}[\mathsf{f}_{\rm m}^{(1)}(\varepsilon)]$ separately, the aforementioned 'appropriate' values for Δ_0, Δ_1, ... will have to be determined self-consistently.

Finally, since the modified SE $\mathsf{f}_{\rm m}^{(1)}(\varepsilon)$ as evaluated within the framework of the SSDA may prove to be an accurate approximation to the exact $\mathsf{f}(\varepsilon)$, one may attempt to determine the 'non-interacting' Hamiltonian underlying this approximation in a self-consistent manner along the lines of (Farid 1997a,b, 1999b).

V. SUMMARY AND CONCLUDING REMARKS

In this work we have determined and presented the four leading terms in the *formal* large-$|\varepsilon|$ AS of the single-particle GF $G_\sigma(\varepsilon)$ and the three leading terms in that of the SE operator $\Sigma_\sigma(\varepsilon)$ pertaining to a system of interacting fermions; for the first-order contribution to the SE in a perturbation series in terms of the *exact* single-particle GF $G_\sigma(\varepsilon)$ pertaining to the *interacting* system and the *exact* dynamically screened interaction function $W(\varepsilon)$, as opposed to the static bare interaction function v, we have determined the *four* leading asymptotic terms for $\Sigma_\sigma(\varepsilon)$. All the indicated terms, which are expressed in terms of *static GS* correlation functions, are amenable to numerical evaluation in terms of GS wavefunctions that are determined within such frameworks as the quantum Monte Carlo method. Each term in the large-$|\varepsilon|$ AS for $\Sigma_\sigma(\varepsilon)$ can be shown to correspond to well-specified contributions in the perturbation series of $\Sigma_\sigma(\varepsilon)$ in terms of v and the *exact* single-particle GF of the *interacting* system, diagrammatically represented by means of skeleton SE diagrams; thus $\Sigma_{\sigma;\infty_0}$, the leading-order term in the large-$|\varepsilon|$ AS for $\Sigma_\sigma(\varepsilon)$, is the *full* contribution of the first-order Hartree and Fock diagrams (which constitute the only first-order skeleton SE diagrams) and $\Sigma_{\sigma;\infty_m}/\varepsilon^m$ (see Eq. (72)), with $m\ge 1$, corresponds to the collection of skeleton diagrams of order p, with $p\in\{2,\dots,m+1\}$ (see specifically §§ III.E.4, 5). On replacing the exact GS correlation functions that feature in the expressions for the coefficients $\Sigma_{\sigma;\infty_m}$, $m=0,1,\dots$ (which in the case of the *exact* SE we have presented in explicit form for $m=0,1$ and 2) by those pertaining to a SSDA of the GS wavefunction of the interacting system, one arrives at highly non-trivial expressions for the mentioned coefficients that qualitatively (and sometimes even quantitatively) reproduce the most essential characteristics of the exact coefficients. This observation unequivocally establishes the crucial significance of skeleton SE diagrams, in comparison with the non-skeleton diagrams, within the framework of many-body perturbation theory. For clarity, with a SSDA for the GS wavefunction is associated a 'non-interacting', or mean-field, many-body Hamiltonian $\widehat{H}_0$ (see Eqs. (54) and (55)), of which the SSD is the GS and which defines the perturbation $\widehat{H}_1{:=}\widehat{H}-\widehat{H}_0$; consequently, the deviation of the SSDA to $\Sigma_{\sigma;\infty_m}$, with $m\ge 0$, from the exact $\Sigma_{\sigma;\infty_m}$ is attributable to the contributions of an *infinite* set of *non*-skeleton proper SE diagrams in terms of $G_{0;\sigma}$ (pertaining to the aforementioned Hamiltonian $\widehat{H}_0$) whose 'skeletons' are the skeleton diagrams of order one when $m=0$ and order p, with $p\in\{2,\dots,m+1\}$, when $m\ge 1$. [103] The influence of these neglected contributions is already apparent from the leading-order term $\Sigma_{\sigma;\infty_0}$ in the large-$|\varepsilon|$ AS of the SE operator in which one encounters the exact GS single-

[103] One should of course also take into account that $\Sigma^{\sharp}_{\sigma;\infty_0}$ (see Eqs. (62) and (72)) is directly dependent on the choice of $\widehat{H}_0$.

particle density matrix ϱ_σ in explicit form (see Eq. (173)); the latter, in contrast with its SSDA counterpart $\varrho_{s;\sigma}$, is strictly *non*-idempotent. That is, whereas $\varrho_{s;\sigma}\varrho_{s;\sigma} \equiv \varrho_{s;\sigma}$, unless $v \equiv 0$, $\varrho_\sigma \varrho_\sigma \not\equiv \varrho_\sigma$.

The asymptotic results for the SE operator can be directly employed in order to obtain accurate and well-controlled approximate results for the energies of the single-particle excitations and the associated wavefunctions (§ III.D) in the regime of 'large' excitation energies. For uniform and isotropic GSs we have *explicitly* established an interplay between the single-particle excitation energies and the value for the average inter-particle distance in the GS and delineated the region where the latter energies can be considered as being 'large' (§ III.E). In this connection it is important to note that, within the framework of the (self-consistent) Hartree-Fock approximation, the single-particle excitation energies are calculated in terms of $\Sigma^{\rm HF}(\boldsymbol{r},\boldsymbol{r}';[\varrho_{s;\sigma}])$ over the *entire* range of these energies; leaving aside the difference between $\varrho_{s;\sigma}$ and ϱ_σ (see above), the fundamental shortcoming of the Hartree-Fock, or indeed *any* static scheme, is already apparent from the absence of such *non-trivial* contribution as $\Sigma_{\sigma;\infty_1}/z$ (see Eq. (72); see also Eqs. (185), (187) and (188)) in the Hartree-Fock SE. We should here emphasize that our *general* considerations in this work are based on the assumption that the interaction potential is such that, for an arbitrary finite value of m, $m \in \{1,2,\dots\}$, $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ is well-defined and bounded for almost *all* $\boldsymbol{r}$ and $\boldsymbol{r}'$. We have, however, explicitly considered the case where $d=3$ and $v \equiv v_c$, the Coulomb potential, for which we have established $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ to be fundamentally unbounded and in need of being regularized (see § II.B) for $m \geq 2$; this regularization is effected through infinite partial summations over specific unbounded terms pertaining to $\Sigma_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ with $p > m$ (note that an unbounded contribution to $\Sigma_{\sigma;\infty_p}(\boldsymbol{r},\boldsymbol{r}')$ can have already been taken account of in the process of regularizing an unbounded term in the expression for $\Sigma_{\sigma;\infty_{m'}}(\boldsymbol{r},\boldsymbol{r}')$ with $m' < m$). It is important to bear in mind the condition $d=3$, since for instance in the case of $d=2$ and Coulomb-interacting fermions, already $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ is fundamentally unbounded and its regularization (see above) gives rise to a term immediately subsequent to $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}') \equiv \Sigma^{\rm HF}(\boldsymbol{r},\boldsymbol{r}';[\varrho_\sigma])$ in a finite-order large-$|\varepsilon|$ AS expansion of $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ that *decays* like $1/|\varepsilon|^{1/2}$ (B. Farid, 2001, unpublished). Evidently, therefore, our statements with regard to Coulomb-interacting fermions both in this Section and in other parts of this paper should *not* be taken as applying to all d; from this perspective it is significant also to recall that the Coulomb potential is not unique in bringing about fundamentally unbounded contributions associated with $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ and needful of regularization. Be it as it may, the appearance of the singular function $(-z/\varepsilon_0)^{1/2}/z$, to be contrasted with $(-z/\varepsilon_0)^{1/2}/z^2$ which corresponds to $d=3$, in the large-$|z|$ AS of $\widetilde{\Sigma}_\sigma(z)$ pertaining to systems of Coulomb-interacting fermions in $d=2$, demonstrates a fundamental hazard inherent in adopting formalisms that are specific to $d=\infty$ and *bounded* v, to applications corresponding to systems of particles interacting through, e.g., $v \equiv v_c$ (see the following paragraph) and finite values of d, specifically $d=2$ and 3. For the case of $v \equiv v_c$ and $d=3$ we explicitly calculate the first *five* leading-order terms in the large-$|z|$ AS for $\widetilde{\Sigma}_\sigma(z)$.

Our investigations concerning the SE operator within the framework of the first-order perturbation theory in terms of the dynamically screened interaction function $W(\varepsilon)$, as opposed to the bare interaction function v, have revealed that, even though this approximation to the SE were to be evaluated in terms of the *exact* single-particle GF $G_\sigma(\varepsilon)$ and the *exact* $W(\varepsilon)$, the resulting expression for $\Sigma_{\sigma;\infty_1}$, the coefficient of the next-to-leading order term in the large-$|\varepsilon|$ AS for $\Sigma_\sigma^{(1)}(\varepsilon)$, would solely consist of a *local* contribution (see Eq. (257) as well as Eq. (259)), in contrast with the *exact* $\Sigma_{\sigma;\infty_1}$ which in addition consists of a non-trivial *non-local* contribution (see Eqs. (185), (187) and (188)). This would not be as severe a shortcoming, were it not that the latter non-local contribution not only implicitly but also *explicitly* depends on the spin state of the single-particle excitations. Further, as our direct calculations show, for systems of fermions in $d=3$ interacting through the Coulomb potential v_c, the next-to-leading term in the large-$|\varepsilon|$ AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ is followed by a *local* term decaying like $1/|\varepsilon|^{3/2}$ for $|\varepsilon| \to \infty$ (to be contrasted with the term decaying like $1/\varepsilon^2$ in the cases where interaction potential is not as singular as the Coulomb potential $v_c(\boldsymbol{r}-\boldsymbol{r}')$ at zero distance [104] and/or cases where the spectrum of the single-particle excitations is bounded from above) which is fundamentally incorrectly described by the SE according to the first-order perturbation theory: compare the expressions in Eqs. (209) and (278) (compare also Eq. (G1) with Eq. (277)). This shortcoming arises because, for $v \rightharpoonup v_c$ in $d=3$, some of the *non*-local contributions to $\Sigma_{\sigma;\infty_2}$ transform into *local* contributions; the first-order perturbation theory taking merely an *incomplete* account of the non-local part of $\Sigma_{\sigma;\infty_2}$ (as we have indicated above, it takes *no* account of the non-local part of $\Sigma_{\sigma;\infty_1}$), it fails to reproduce, even approximately, the local contributions as arising from non-local ones in $\Sigma_{\sigma;\infty_2}$ in consequence of the transformation $v \rightharpoonup v_c$. In addition to showing a main shortcoming of $\Sigma_\sigma'^{(1)}(\varepsilon)$ (see Eq. (241)), this observation unequivocally demonstrates that a dynamical local approximation to the SE operator

[104] The long range of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ for $\|\boldsymbol{r}-\boldsymbol{r}'\| \to \infty$ brings about a contribution proportional to $\ln(-z/\varepsilon_0)/z^2$, with $z = \varepsilon \pm i\eta$, $\eta \downarrow 0$, for $\varepsilon \to \pm\infty$ (see Eqs. (213) and (F160)).

that proves *accurate* for systems of particles interacting through $v \not\equiv v_c$, is necessarily *less accurate* when v is identified with v_c. This finding is specifically relevant in connection with the so-called 'dynamical mean-field approximation' (for a review see Georges, *et al.* 1996) to the SE operator which has found application in *ab initio* calculations in real materials and is referred to as 'LDA^{++}' (Lichtenstein and Katsnelson 1998, Katsnelson and Lichtenstein 2000); although the SE employed in this approach is ε-dependent, it is purely *local*; it has its origin in the solution of the single-impurity Anderson (1961) problem and is related to the SE of the Hubbard model through the equivalence (Ohkawa 1991, Georges and Kotliar 1992) of the former with the latter in $d = \infty$ (Metzner and Vollhardt 1989). Our considerations unambiguously show that, whereas the 'dynamical mean-field approximation' to the SE operator may be accurate while dealing with the Hubbard Hamiltonian corresponding to a finite d (in particular to $d = 2, 3$), it necessarily provides a less accurate description of the exact SE operator in systems where the inter-particle interaction is the Coulomb interaction. In this connection note that, in dealing with the Hubbard Hamiltonian, one has to deal with an intra-atomic particle-particle interaction potential that in stark contrast with the Coulomb potential v_c is both bounded and localized. For a discussion of the limitations of the 'dynamical mean-field approximation' from the standpoint of other authors (ours is *exclusively* based on our observations in the present paper) see the review article by Georges, *et al.* (1996, § IX).

We have put forward a practicable formalism (see § IV.D) that overcomes the shortcomings of the first-order SE operator (in terms of W) at large values of $|\varepsilon|$. The modified SE (see Eq. (281)) is applicable for *all* values of ε and, in view of its built-in correct asymptotic behaviour for $|\varepsilon| \to \infty$, is related to a single-particle spectral function $A_\sigma(\varepsilon)$ whose ε moments integrals (to some finite order, depending on the number of terms in the large-$|\varepsilon|$ AS of the exact SE the modified SE is designed exactly to reproduce; see Eq. (281)) are *identical* with those of the *exact* $A_\sigma(\varepsilon)$ (see § III.B).

One of the consequences of the aforementioned misrepresentation of the SE within the framework of the first-order perturbation theory is that, according to this approximate theory, magnetism in its various forms is, roughly speaking, driven by 'secondary' effects, as the SE in this framework does *not* give due prominence to the *explicit* dependence of the exact SE on the spin indices of the single-particle excitations. The relevance of this observation can be appreciated by recalling the early discussions concerning the occurrence of ferromagnetism in transition metal compounds and the corresponding deriving mechanisms (Slater 1953, Wohlfarth 1953, van Vleck 1953), while bearing in mind that the *explicit* dependence of $\Sigma^{\text{HF}}[\varrho_\sigma] \equiv \Sigma_{\sigma;\infty_0}[\varrho_\sigma]$ (see Eq. (173)) upon σ is solely through ϱ_σ (in practice, through $\varrho_{\text{s};\sigma}$ calculated self-consistently) and that, according to the current understanding of the subject (see also the following paragraph), 'correlation' (as distinct from 'exchange') is an essential aspect of magnetism in the indicated compounds (for example Fulde (1991)).

Concerning the relevance of the *explicit* dependence on σ of the exact $\Sigma_\sigma(\varepsilon)$, Harris and Lange (1967) observed that *"in addition to band narrowing, one should include the spin-dependent shifts in the band energy which favor ferromagnetism when discussing questions of magnetic stability."* Harris and Lange (1967) further observed that *"the electron excitations have a longer lifetime in the paramagnetic phase than in the antiferromagnetic phase"*, which is in full conformity with our finding that the coefficient of the term in the large-$|\varepsilon|$ AS of $\Sigma_\sigma(\varepsilon)$ that decays like $1/|\varepsilon|^{3/2}$ is *identically* vanishing when the distribution of the spin-σ (read 'spin-$\uparrow$' for electrons) particles is in *local* balance with that of the spin-$\bar{\sigma}$ (read 'spin-$\downarrow$' for electrons) particles (see Eqs. (G7) and (G15)). This aspect is appreciated by considering the fact that the appearance of a term in the large-$|\varepsilon|$ AS for $\Sigma_\sigma(\varepsilon)$ decaying like $1/|\varepsilon|^{3/2}$, there where a term decaying like $1/\varepsilon^2$, *or* like $\ln(|\varepsilon/\varepsilon_0|)/\varepsilon^2$, would be expected, amounts to a broadening of the single-particle spectral function (compare cases (I) and (II) in Eq. (239)). We point out that the term decaying like $1/|\varepsilon|^{3/2}$ owes its existence to the short-range part of the Coulomb interaction function (see § III.H.2). It is important to realize that this observation and that by Harris and Lange (1967) based on investigations corresponding to the Hubbard Hamiltonian (involving a *bounded* intra-atomic interaction), quoted above, do *not* imply contradiction, for in our considerations we have dealt with systems with unbounded single-particle spectra, while in the case of the Hubbard model considered by Harris and Lange (1967), the single-particle spectrum is bounded. Consequently (see § I.C), in the former case the single-particle spectral function $A_\sigma(\varepsilon)$ has an unbounded support, whereas in the latter case this function has a bounded support for which a *finite*-order AS representation in terms of the sequence $\{1, 1/\varepsilon, 1/\varepsilon^2, \dots\}$, similar to that presented in Eq. (239), *cannot* suffice. In this connection, recall that (see § II.B) the sequence $\{1, 1/\varepsilon, 1/\varepsilon^2, \dots\}$ is an asymptotic one in the region $|\varepsilon| \to \infty$.

While dealing with the large-$|\varepsilon|$ asymptotic behaviour of the single-particle spectral function $\overline{A}_\sigma(k;\varepsilon)$ pertaining to uniform and isotropic GSs (see § III.I), we have emphasized the significance of inhomogeneity in GSs and the non-trivial influence of this (through, e.g., the Umklapp processes in periodic crystals) on the relationship between the SE operator and the single-particle spectral function. In particular, in such systems it is *not* possible to deduce the diagonal elements of the self-energy operator in the momentum representation solely from those of the single-particle spectral function (and vice versa) as measured by means of angle-resolved photo-emission and inverse photo-emission spectroscopy, *not even* in the regime of large transfer energies. Consequently, any attempt to model the diagonal elements of the self-energy operator in the momentum space, entirely on the basis of the measured diagonal elements of the single-particle spectral function of inhomogeneous systems, is *a priori* doomed to be inaccurate, not only quantitatively, but also qualitatively.

Our considerations have led us to a further conclusion which to our knowledge has never earlier been drawn in other works. In order to present this conclusion, we need first to provide some background detail. To this end consider the many-body perturbation series for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ in terms of the *bare* particle-particle interaction function v and the skeleton SE diagrams. For definiteness consider $d=3$. It is well-known that for metallic GSs and $v \equiv v_c$, this series involves *unbounded* contributions, arising from the long range of v_c (for example Mattuck (1992, § 10.4)); [105] these unbounded contributions are eliminated through expressing the perturbation series in terms of the *screened* interaction function $W(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (see Eq. (242)) which, in contrast with the bare interaction function v_c, is dependent on ε. On the other hand, to our knowledge for systems whose GSs are non-metallic, *no* unbounded contributions in the above-mentioned perturbation series had been expected thus far, so that for these systems the series in terms of v_c is universally believed to be well-defined. [106] The interesting conclusion to which we have just referred is that the mentioned perturbation series, in terms of the bare v_c, is in fact ill-defined *even* for the latter systems (see the last two paragraphs of § III.H.2). We have arrived at this conclusion through the observation that for $v \equiv v_c$ and $d=3$, the coefficient of $1/\varepsilon^2$, i.e. $\Sigma_{\sigma;\infty_2}$, involves unbounded contributions arising from *both* the long range of v_c *and* its specific form of divergence at the origin; [107] in order to retain a well-defined finite-order AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ corresponding to $|\varepsilon| \to \infty$, it is *necessary* to perform partial summations over *infinite* number of specific contributions pertaining to $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, $m=2,3,4,\ldots$. The necessity for performing such summations (here particularly owing to the specific behaviour of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ for $\|\boldsymbol{r}-\boldsymbol{r}'\| \to 0$), irrespective of the nature of the GS, whether metallic or otherwise, makes evident that a *finite*-order perturbation series in terms of the bare v does *not* suffice in cases where $v \equiv v_c$ and $d=3$, even for systems with non-metallic GSs (§ II.B).

Performing, for $v \equiv v_c$ and $d=3$, the above-mentioned infinite partial summations, we have obtained that, in the large-$|\varepsilon|$ AS for $\Sigma_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$, $\Sigma^{\text{HF}}(\boldsymbol{r},\boldsymbol{r}';[\varrho_\sigma]) + \Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')/\varepsilon$ is followed by contributions that decay like $1/|\varepsilon|^{3/2}$, $\ln(|\varepsilon/\varepsilon_0|)/\varepsilon^2$, $1/\varepsilon^2$, $\ldots$, rather than merely $1/\varepsilon^2$, $\ldots$ as would be expected from the *formal* structure of the AS for the SE corresponding to short-range and bounded interaction functions v (see Eq. (72)). In addition, we have deduced that $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ involves a contribution proportional to $v^3(\boldsymbol{r}-\boldsymbol{r}')$ which, although well-defined in the case of $v \equiv v_c$ in $d=3$, is *not* integrable, implying (see § II.B) an associated fundamentally unbounded contribution in the momentum representation of $\Sigma_{\sigma;\infty_2}$. We have resolved this problem through a further summation over an infinite number of pertinent non-integrable contributions pertaining to $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, with $m \geq 2$, and deduced an *additional* singular contribution of the form $\ln(|\varepsilon/\varepsilon_0|)/\varepsilon^2$ to the AS of the momentum representation of $\Sigma_\sigma(\varepsilon)$ for $|\varepsilon| \to \infty$. We observe that the most dominant singular contribution to a finite-order AS of $\widetilde{\Sigma}_\sigma(z)$ for $|z| \to \infty$ in the cases corresponding to $v \equiv v_c$ in $d=3$, both in the coordinate representation and in the momentum representation, is proportional to $(-z/\varepsilon_0)^{1/2}/z^2$ which has its origin in the specific behaviour of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ for $\|\boldsymbol{r}-\boldsymbol{r}'\| \to 0$ (the existence of this contribution also vitally depends on the single-particle excitation spectra being unbounded from above). Importantly, this singular contribution in a finite-order large-$|z|$ AS for $\widetilde{\Sigma}_\sigma(z)$ owes its existence to the number density of particles with spin index σ being in at least local *imbalance* with the total number density of the remaining particles in the system (see footnote 107).

The appearance of functions with branch-cut singularity in the AS expansion of $\widetilde{\Sigma}_\sigma(z)$ for $|z| \to \infty$, such as $(-z/\varepsilon_0)^{1/2}/z^2$ and $\ln(-z/\varepsilon_0)/z^2$ (see § III.H), implies not only that $\widetilde{\Sigma}_\sigma(z)$ possesses a manifold of branch-point singularities at the point of infinity in the complex z plane, but also that $\widetilde{\Sigma}_\sigma(z)$ must possess associated branch-point singularities in the *finite* part of the z plane. Since with the exclusion of the real energy axis, $\widetilde{\Sigma}_\sigma(z)$ is analytic everywhere on the complex z plane, it follows that the latter branch-point singularities must be located on the finite part of the real energy axis. Knowledge of the location of each of these points, say ε_j, together with that of the associated singular function in the AS of $\widetilde{\Sigma}_\sigma(z)$, for $|z| \to \infty$, is sufficient partially to uncover the behaviour of $\widetilde{\Sigma}_\sigma(z)$ for $|z-\varepsilon_j| \to 0$. This aspect is of particular significance in the case of systems with metallic GSs where the coincidence of ε_j (and possibly other singular points) with the Fermi energy ε_F of the system provides one with

[105] These unbounded contributions correspond to the set of polarization diagrams that constitute the RPA to the polarization function.

[106] A 'well-defined' perturbation series is *not* necessarily convergent.

[107] Our calculations show that the divergence of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ for $\|\boldsymbol{r}-\boldsymbol{r}'\| \to 0$ plays a role in cases where $n_\sigma(\boldsymbol{r}) \not\equiv n_{\bar{\sigma}}(\boldsymbol{r})$, where $n_{\bar{\sigma}}(\boldsymbol{r})$ stands for the *total* number density of fermions with the exclusion of those associated with the spin index σ (see Eqs. (163) and (164)); in the case of spin-1/2 fermions, $\bar{\sigma} = -\sigma$ so that $n_{\bar{\sigma}}(\boldsymbol{r}) \equiv n_{-\sigma}(\boldsymbol{r})$.

information of potentially considerable significance (this depending on the singular function at issue) concerning the nature of the underlying metallic state (see § I.B). In this connection it is important to realize that determination of the terms in the AS of $\widetilde{\Sigma}_\sigma(z)$ pertinent to $|z| \to \infty$ is significantly less demanding than that of the terms in the AS of $\widetilde{\Sigma}_\sigma(z)$ appropriate to $|z - \varepsilon_F| \to 0$. Consequently, although to our knowledge there exists no *a priori* reason for the coincidence of the Fermi energy of systems with metallic GSs with one or some of the counterparts of the singularities of $\widetilde{\Sigma}_\sigma(z)$ at the point of infinity of the z plane (see footnote 12; although there *may* be conditions, as yet to be established, under which such coincidence would become unavoidable), it is nonetheless advantageous to establish the singular behaviour of $\widetilde{\Sigma}_\sigma(z)$ for $|z| \to \infty$ in considerations that primarily are concerned with the behaviour of $\widetilde{\Sigma}_\sigma(z)$ for $|z - \varepsilon_F| \to 0$; knowledge of the behaviour of $\widetilde{\Sigma}_\sigma(z)$ for $|z| \to \infty$ provides one with much valuable information not only concerning the single-particle excitations at high excitation energies (§ III.E) but also, through the interplay between the latter and the energy moments integrals of the single-particle spectral function $A_\sigma(\varepsilon)$ (see § III.B), concerning the positions, widths and other aspects of the prominent peaks in $A_\sigma(\varepsilon)$.

Finally, although our attention in the present work has been mainly centred around the single-particle GF and the SE operator, much of our considerations are directly applicable to other dynamical correlation functions pertaining to interacting systems. Of these, to name but two, one is the dynamical density-density response function (see Engel and Farid 1993), which has featured in our investigations through the dynamically screened interaction function $W(\varepsilon)$ (see § IV), and the dynamical spin-spin correlation function, which although it is related to the latter response function (see footnote 99), has *not* appeared as prominently as $W(\varepsilon)$ in the foreground of our discussions. In particular we should like to emphasize that the scheme proposed in § IV.D for removing the shortcomings of an approximation to the SE operator, can be trivially extended for improving the approximate expressions for any of the above-mentioned dynamical correlation functions; one may think of these approximate expressions as being those according to the RPA of these functions.

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Note added in proof. It has very recently come to our attention that Deisz, *et al.* (1997) have explicitly demonstrated that for large $|\varepsilon|$, the exact $1/\varepsilon$ dependence of the self-energy pertaining to the single-band Hubbard Hamiltonian is entirely determined by the second-order skeleton self-energy diagram evaluated in terms of the exact single-particle Green function. Our findings (see §§ I.B, III.E, III.H and V) not only conform with this result, but they reveal an intimate relationship between $\Sigma_{\sigma;\infty_m}$ (the coefficient corresponding to the $1/\varepsilon^m$ term, $\forall m$, in the large-$|\varepsilon|$ asymptotic series of $\Sigma_\sigma(\varepsilon)$ pertaining to a *general* Hamiltonian) and specific sets of skeleton self-energy diagrams.

Further, the coefficient of $1/\varepsilon^2$ on the RHS of Eq. (227) can be *simplified* by absorbing the term $2\Sigma_{\sigma;\infty_1}/\Delta$ in the ε' integral. Upon this, through the same line of reasoning as presented in the paragraph preceding Eq. (227), for the coefficient of $1/\varepsilon^2$ on the RHS of Eq. (227), that is Π_σ (see the text following equation Eq. (234)), we obtain

$$\Pi_\sigma = -\wp \int_0^\infty \frac{\mathrm{d}\varepsilon'}{\varepsilon'^3} \Big\{ \mathrm{Re}\Sigma_\sigma(1/\varepsilon') - \mathrm{Re}\Sigma_\sigma(-1/\varepsilon') - 2\varepsilon'\, \Sigma_{\sigma;\infty_1} \Big\}.$$

□

APPENDICES

APPENDIX A: NON-ORTHOGONALITY AND OVER-COMPLETENESS OF THE SET OF LEHMANN AMPLITUDES

Here we demonstrate that, for systems of interacting fermions, the Lehmann amplitudes $\{f_{s;\sigma}(\boldsymbol{r})\}$ as defined in Eq. (18) do *not* form an orthonormal set. This, together with the fact that $\{f_{s;\sigma}(\boldsymbol{r})\}$ satisfies the closure relation (see Eq. (30)), establishes the *over-completeness* of the set of the Lehmann amplitudes. This aspect is important for a proper understanding of the nature of the single-particle excitations in interacting systems in particular it sheds light on the significance of Eq. (42). In § A.2, by employing a number of the general results of § A.1, we deduce a simple approximate expression for the dispersion of the single-particle excitation energies in uniform systems. This provides us with an opportunity to view some of the abstract concepts of § A.1 in a more applied context.

1. Basic considerations; the overcompleteness

Consider the 'non-interacting' Hamiltonian $\widehat{H}_0$ in Eq. (54) with the single-particle Hamiltonian $h_{0;\sigma}(\boldsymbol{r})$ defined in Eq. (55). Let $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$ be the *complete* set of orthonormal eigenfunctions of $h_{0;\sigma}(\boldsymbol{r})$ (see Eq. (56)). [108] Completeness implies the closure relation

$$\sum_{\varsigma} \varphi^*_{\varsigma;\sigma}(\boldsymbol{r})\varphi_{\varsigma;\sigma}(\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{A1}$$

With $\hat{\mathsf{a}}_{\varsigma;\sigma}$ the fermion annihilation operator corresponding to $\varphi_{\varsigma;\sigma}(\boldsymbol{r})$, satisfying (*cf.* Eq. (91))

$$\begin{aligned}&\big[\hat{\mathsf{a}}^{\dagger}_{\varsigma;\sigma}, \hat{\mathsf{a}}_{\varsigma';\sigma'}\big]_+ = \delta_{\sigma,\sigma'}\,\delta_{\varsigma,\varsigma'},\\ &\big[\hat{\mathsf{a}}^{\dagger}_{\varsigma;\sigma}, \hat{\mathsf{a}}^{\dagger}_{\varsigma';\sigma'}\big]_+ = \big[\hat{\mathsf{a}}_{\varsigma;\sigma}, \hat{\mathsf{a}}_{\varsigma';\sigma'}\big]_+ = 0,\end{aligned} \tag{A2}$$

we have the following representation for the annihilation field operator $\hat{\psi}_\sigma(\boldsymbol{r})$:

$$\hat{\psi}_\sigma(\boldsymbol{r}) = \sum_{\varsigma} \hat{\mathsf{a}}_{\varsigma;\sigma}\,\varphi_{\varsigma;\sigma}(\boldsymbol{r}). \tag{A3}$$

From the definition for the Lehmann amplitudes in Eq. (18) we thus deduce that

$$f_{s;\sigma}(\boldsymbol{r}) = \sum_{\varsigma} \chi_{s;\sigma}(\varsigma)\,\varphi_{\varsigma;\sigma}(\boldsymbol{r}), \tag{A4}$$

where

$$\chi_{s;\sigma}(\varsigma) {:=} \begin{cases} \langle\Psi_{N_\sigma-1,N_{\bar\sigma};s}|\hat{\mathsf{a}}_{\varsigma;\sigma}|\Psi_{N;0}\rangle, & \varepsilon_{s;\sigma} < \mu,\\[6pt] \langle\Psi_{N;0}|\hat{\mathsf{a}}_{\varsigma;\sigma}|\Psi_{N_\sigma+1,N_{\bar\sigma};s}\rangle, & \varepsilon_{s;\sigma} > \mu.\end{cases} \tag{A5}$$

Thus we have

$$S_{s,s'} {:=} \int \mathrm{d}^d r\; f^*_{s;\sigma}(\boldsymbol{r}) f_{s';\sigma}(\boldsymbol{r}) = \sum_{\varsigma} \chi^*_{s;\sigma}(\varsigma)\chi_{s';\sigma}(\varsigma). \tag{A6}$$

Let now $\mathsf{n}_\sigma(\varsigma)$ be the GS distribution function corresponding to the particles associated with $\{\hat{\mathsf{a}}_{\varsigma;\sigma}\}$, defined as (*cf.* Eq. (J2))

$$\mathsf{n}_\sigma(\varsigma) {:=} \langle\Psi_{N;0}|\hat{\mathsf{a}}^{\dagger}_{\varsigma;\sigma}\hat{\mathsf{a}}_{\varsigma;\sigma}|\Psi_{N;0}\rangle. \tag{A7}$$

With

$$\nu_\sigma(\varsigma) {:=} \begin{cases} \mathsf{n}_\sigma(\varsigma), & \varepsilon_{s;\sigma} < \mu,\\ 1-\mathsf{n}_\sigma(\varsigma), & \varepsilon_{s;\sigma} > \mu,\end{cases} \tag{A8}$$

for $\nu_\sigma(\varsigma) \neq 0$, we define

$$|\Psi^0_{N_\sigma-1,N_{\bar\sigma};\varsigma}\rangle {:=} \frac{1}{\sqrt{\nu_\sigma(\varsigma)}}\,\hat{\mathsf{a}}_{\varsigma;\sigma}|\Psi_{N;0}\rangle, \tag{A9}$$

$$|\Psi^0_{N_\sigma+1,N_{\bar\sigma};\varsigma}\rangle {:=} \frac{1}{\sqrt{\nu_\sigma(\varsigma)}}\,\hat{\mathsf{a}}^{\dagger}_{\varsigma;\sigma}|\Psi_{N;0}\rangle. \tag{A10}$$

It can be readily verified that the state vectors defined in Eqs. (A9) and (A10) are normalized to unity and moreover are eigenstates of the *partial* number operators $\widehat{N}_\sigma$, $\sigma = -\mathsf{s}, -\mathsf{s}{+}1, \dots, \mathsf{s}$, corresponding respectively to $N_\sigma - 1$ and $N_\sigma + 1$ particles with spin σ.

Making use of the completeness of $\{|\Psi_{N_\sigma-1,N_{\bar\sigma};s}\rangle\}$ and $\{|\Psi_{N_\sigma+1,N_{\bar\sigma};s}\rangle\}$ in the $(N_\sigma - 1 + N_{\bar\sigma})$- and $(N_\sigma + 1 + N_{\bar\sigma})$-particle subspaces respectively of the Fock space (see Eq. (31)), one can write

$$|\Psi^0_{N_\sigma\pm1,N_{\bar\sigma};\varsigma}\rangle = \sum_{s} \gamma^{\pm}_{s;\sigma}(\varsigma)|\Psi_{N_\sigma\pm1,N_{\bar\sigma};s}\rangle, \tag{A11}$$

from which, following the normalization to unity of the state vectors on both sides of Eq. (A11), one obtains

$$\sum_{s} |\gamma^{\pm}_{s;\sigma}(\varsigma)|^2 \equiv 1, \quad \forall\,\varsigma. \tag{A12}$$

Rewriting Eq. (A9) as

$$\hat{\mathsf{a}}_{\varsigma;\sigma}|\Psi_{N;0}\rangle = \sqrt{\nu_\sigma(\varsigma)}\,|\Psi^0_{N_\sigma-1,N_{\bar\sigma};\varsigma}\rangle$$

and Eq. (A10) as

$$\langle\Psi_{N;0}|\hat{\mathsf{a}}_{\varsigma;\sigma} = \sqrt{\nu_\sigma(\varsigma)}\,\langle\Psi^0_{N_\sigma+1,N_{\bar\sigma};\varsigma}|,$$

from Eq. (A5), making use of the representation in Eq. (A11) together with the orthonormality property $\langle\Psi_{N_\sigma\pm1,N_{\bar\sigma};s}|\Psi_{N_\sigma\pm1,N_{\bar\sigma};s'}\rangle = \delta_{s,s'}$, it readily follows that

[108] The considerations of this Appendix could have been based on any *complete* and orthonormal set of one-particle orbitals (note that 'completeness' implies, among other things, compatibility with the single-particle Hilbert space of the problem at hand), notably $\{\phi_\varsigma(\boldsymbol{r})\}$, the orthonormal set of eigenfunctions of the non-interacting single-particle Hamiltonian $h_0(\boldsymbol{r})$ defined in Eq. (43) (see Eq. (44)). The drawback of employing any other complete set than $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$ would be to deprive ourselves of the ability to relate our results to a 'non-interacting' system and thereby of the possibility to attribute certain properties to 'interaction'. Although viewed from this perspective, it would appear that the choice of $\{\phi_\varsigma(\boldsymbol{r})\}$ would be more appropriate, and although in certain cases the choice between $\{\phi_\varsigma(\boldsymbol{r})\}$ and $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$ can be immaterial, *in general* the GS of the truly non-interacting Hamiltonian $\widehat{H}_0 = \widehat{T} + \widehat{U}$ (see Eq. (1)), corresponding to $h_0(\boldsymbol{r})$, is *not* adiabatically connected with that of the fully interacting Hamiltonian (see § III.C, in particular the paragraph following that containing Eq. (61)). Consequently, in such cases any reference to 'interaction effects' would be spurious, for the adiabatic evolution of the GS of the $\widehat{H}_0$ through the adiabatic 'switching on' of $\widehat{V}$ (see Eq. (1)) would not lead to the true GS of $\widehat{H}$ but to some other eigenstate. It follows that the choice of $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$ is far superior than that of $\{\phi_\varsigma(\boldsymbol{r})\}$. It is significant to realize that (see Eq. (56) and the subsequent discussions) by reducing the value of the coupling constant of the particle-particle interaction, the set $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$ naturally reduces to $\{\phi_\varsigma(\boldsymbol{r})\}$ so that our results in this Appendix also retain a natural connection with the truly non-interacting system described by $\widehat{T} + \widehat{U}$.

$$\chi_{s;\sigma}(\varsigma) = \begin{cases} \sqrt{\nu_\sigma(\varsigma)}\, \gamma^{-}_{s;\sigma}(\varsigma), & \varepsilon_{s;\sigma} < \mu, \\ \sqrt{\nu_\sigma(\varsigma)}\, \gamma^{+*}_{s;\sigma}(\varsigma), & \varepsilon_{s;\sigma} > \mu, \end{cases} \tag{A13}$$

from which we deduce that

$$\sum_{\varsigma} \chi^*_{s;\sigma}(\varsigma)\chi_{s;\sigma}(\varsigma) = \sum_{\varsigma} \nu_\sigma(\varsigma)\, |\gamma^{\mp}_{s;\sigma}(\varsigma)|^2, \;\; \varepsilon_{s;\sigma} \lessgtr \mu. \tag{A14}$$

The case corresponding to $s \neq s'$, involving *four* possibilities associated with the four combinations ($\varepsilon_{s;\sigma} < \mu, \varepsilon_{s';\sigma} < \mu$), ($\varepsilon_{s;\sigma} < \mu, \varepsilon_{s';\sigma} > \mu$), etc., can be easily dealt with; however, we shall not consider these in this Appendix.

From $\langle\Psi_{N_\sigma\pm1,N_{\bar\sigma};s}|\Psi_{N_\sigma\pm1,N_{\bar\sigma};s'}\rangle = \delta_{s,s'}$ and Eq. (A11) we have (*cf.* Eq. (A12))

$$\sum_{\varsigma} |\gamma^{\pm}_{s;\sigma}(\varsigma)|^2 = \langle\Psi_{N_\sigma\pm1,N_{\bar\sigma};s}| \times\Big(\sum_{\varsigma} |\Psi^0_{N_\sigma\pm1,N_{\bar\sigma};\varsigma}\rangle\langle\Psi^0_{N_\sigma\pm1,N_{\bar\sigma};\varsigma}|\Big)|\Psi_{N_\sigma\pm1,N_{\bar\sigma};s}\rangle = 1, \quad \forall\, s, \tag{A15}$$

where we have made use of the fact that the projection operator on the RHS of Eq. (A15), enclosed by large parentheses, can be replaced by the unit operator I (and that $|\Psi_{N_\sigma\pm1,N_{\bar\sigma};s}\rangle$ are normalized to unity). It is important to note that although in the case of interacting systems the compound variable ς associated with the states defined in Eqs. (A9) and (A10) belongs to a *proper* subset of the set to which the compound variable s belongs, [109] implying that in general

$$\langle\Psi^0_{N_\sigma\pm1,N_{\bar\sigma};\varsigma}|\widehat{H}|\Psi^0_{N_\sigma\pm1,N_{\bar\sigma};\varsigma'}\rangle \neq 0, \;\; \text{for } \varsigma \neq \varsigma', \tag{A16}$$

nonetheless, $\{|\Psi^0_{N_\sigma\pm1,N_{\bar\sigma};\varsigma}\rangle\}$ is *complete* within the Hilbert spaces of the $(N_\sigma \pm 1 + N_{\bar\sigma})$-particle states; the indicated difference between the nature of the variables s and ς reflects the *over-completeness* of the set $\{|\Psi_{N_\sigma\pm1,N_{\bar\sigma};s}\rangle\}$ within the above-mentioned Hilbert spaces. This over-completeness implies that the overlap matrix $\boldsymbol{S}$, whose (s,s') component is defined in Eq. (A6), is defective, that is $\det[\boldsymbol{S}] = 0$.

For *'non-interacting'* systems, [110] we have (*cf.* Eq. (A11))

$$\gamma^{\mp}_{s;\sigma}(\varsigma) = \delta_{s,\varsigma}, \quad \nu_\sigma(\varsigma) = 1, \tag{A17}$$

from which, in conjunction with Eqs. (A13) and (A6), it follows that $\int \mathrm{d}^d r\, f^*_{s;\sigma}(\boldsymbol{r}) f_{s;\sigma}(\boldsymbol{r}) = 1$ where $f_{s;\sigma}(\boldsymbol{r}) \equiv \varphi_{\varsigma;\sigma}(\boldsymbol{r})$ (note that, as our notation involving $\delta_{s,\varsigma}$ makes explicit, here the variables s and ς are elements of the same set; see text following Eq. (48)).

For *interacting* systems, we have [111]

$$0 \le \nu_\sigma(\varsigma) \le 1 \quad \text{and} \quad \exists\varsigma \;\text{ for which }\; \nu_\sigma(\varsigma) \neq 1, \tag{A18}$$

from which and Eq. (A15) it follows that

$$\sum_{\varsigma} \nu_\sigma(\varsigma)|\gamma^{\mp}_{s;\sigma}(\varsigma)|^2 < \sum_{\varsigma} |\gamma^{\mp}_{s;\sigma}(\varsigma)|^2 = 1, \quad \text{for } \textit{some } s, \tag{A19}$$

which implies, through Eqs. (A6) and (A14), that for *interacting* systems we must have

$$\int \mathrm{d}^d r\; f^*_{s;\sigma}(\boldsymbol{r})\, f_{s;\sigma}(\boldsymbol{r}) < 1, \;\; \text{for } \textit{some } s. \tag{A20}$$

This demonstrates that, for interacting systems, $\{f_{s;\sigma}(\boldsymbol{r})\}$ is *not* normalized to unity for *some*, if not all (see footnote 111), s. With reference to our qualification 'some', we point out that, if for a *given* s, say s_0, $\gamma^{\mp}_{s_0;\sigma}(\varsigma)$ happens to be vanishing *exclusively* for a non-empty set S_0 of ς values for which

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[109] Following Klein and Prange (1958) (see footnote 14 and the text following Eq. (51) herein), we may write $s = (\varsigma, \alpha)$ where α stands for a "parameter of degeneracy", distinguishing various states corresponding to a given ς. It is this extension of the parameter space required for marking the $(N\pm1)$-particle eigenstates of $\widehat{H}$ (with the N-particle GS as the reference state), in comparison with that required for marking a complete basis set for the single-particle Hilbert state of the problem, that gives rise to the over-completeness of $\{f_{s;\sigma}(\boldsymbol{r})\}$. As we have pointed out in footnote 50, the designation "parameter of degeneracy" does not appropriately reflect the true significance of α.

[110] In this case, all state vectors that in our above considerations have involved Ψ (such as $|\Psi_{N_\sigma\pm1,N_{\bar\sigma};s}\rangle$, etc.), should be viewed as having been replaced by their non-interacting counterparts involving Φ (such as $|\Phi_{N_\sigma\pm1,N_{\bar\sigma};\varsigma}\rangle$, etc.). See footnote 108 for the basic property required from 'non-interacting' systems.

[111] Consider uniform and isotropic systems of interacting spin-1/2 fermions in $d = 3$. The fact that for these systems $0 < \mathsf{n}_\sigma(k) < 1$, $\forall k$, so that $0 < \nu_\sigma(k) < 1$, $\forall k$, implies that for the case at hand *all* the following uses of the word 'some' are in fact to be replaced by the word 'all'. Most importantly, for these systems $\int \mathrm{d}^d r\; f^*_{s;\sigma}(\boldsymbol{r}) f_{s;\sigma}(\boldsymbol{r}) < 1$ for *all* s (*cf.* Eq. (A20)). It has to be noted, however, that the rapid decay of $\mathsf{n}(k)$ for $k \to \infty$ as presented in Eq. (J4) (see also the text following this equation) and consequently the rapid approach of the corresponding $\nu(k) \equiv \sum_{\sigma=\uparrow,\downarrow} \nu_\sigma(k)$ towards unity (see Eq. (A8)) as $k \to \infty$, is indicative of the fact that, for $\varepsilon_{s;\sigma}$ larger than a small multiple of ε_F (say, larger than twice to three times ε_F), to a very good approximation $\int \mathrm{d}^d r\; f^*_{s;\sigma}(\boldsymbol{r}) f_{s;\sigma}(\boldsymbol{r})$ can be identified with unity (*cf.* Eq. (48) above). This in turn specifies the range of ε above which $\mathrm{Im}[\overline{\Sigma}_\sigma(k;\varepsilon)]$ can be considered as being negligible.

$\nu_\sigma(\varsigma) \neq 1$, then $\sum_\varsigma \nu_\sigma(\varsigma)|\gamma^{\mp}_{s_0;\sigma}(\varsigma)|^2 = 1$ obtains and thus $\int \mathrm{d}^d r\, f^*_{s_0;\sigma}(\boldsymbol{r}) f_{s_0;\sigma}(\boldsymbol{r}) = 1$; evidently, however, since $\gamma^{\mp}_{s;\sigma}(\varsigma)|_{\varsigma\in S_0} = 0$ *cannot* be valid for *all* s, for otherwise Eq. (A12) would be violated, it follows that $f_{s;\sigma}(\boldsymbol{r})$ *cannot* be of unit norm for *all* s. In contrast, the independence of $\nu_\sigma(\varsigma)$ from s implies that the possibility of $\int \mathrm{d}^d r\, f^*_{s;\sigma}(\boldsymbol{r}) f_{s;\sigma}(\boldsymbol{r}) = 1$ for some s must be a matter of accident, so that in general and so long as $v \not\equiv 0$, the word '*some*' in Eq. (A20) should be interchangeable with the word '*all*'.

Along the same lines as above, one can demonstrate that $\{f_{s;\sigma}(\boldsymbol{r})\}$ is *not* orthogonal for interacting systems. It is important to realize that the observation that for *interacting* systems the norm of $f_{s;\sigma}(\boldsymbol{r})$ is *less* than unity (for *some*, if not *all*, s) conforms with the fact that, while for interacting systems the compound variable ς belongs to a *proper* subset of the set to which the compound variable s belongs, nonetheless both $\{f_{s;\sigma}(\boldsymbol{r})\}$ and $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$ satisfy the closure relation as presented in Eqs. (30) and (A1) respectively.

To close our above discussion, we proceed by briefly elaborating on the over-completeness of $\{f_{s;\sigma}(\boldsymbol{r})\}$ in the case of $v \not\equiv 0$. For definiteness, consider a case where $h_{0;\sigma}(\boldsymbol{r})$ or, what is the same, $u(\boldsymbol{r})+w_\sigma(\boldsymbol{r})$, is invariant under the operations of some (discrete or continuous) symmetry group. From this it follows that $\{\varphi_{\varsigma;\sigma}(\boldsymbol{r})\}$ can be arranged to form the basis for the unitary irreducible representations of the underlying symmetry group. By doing this, a specific index ς identifies $\varphi_{\varsigma;\sigma}(\boldsymbol{r})$ with one specific basis function pertaining to one specific unitary irreducible representation of a general representation of the symmetry group of $h_{0;\sigma}(\boldsymbol{r})$ (for example Cornwell (1984, pp. 81-83)). Thus for instance, by assuming $u(\boldsymbol{r})+w_\sigma(\boldsymbol{r})$ to be invariant under a discrete translation group, we can write $\varsigma = (\boldsymbol{k}, \ell)$, where $\boldsymbol{k}$ stands for a point inside the first Brillouin zone corresponding to the underlying Bravais lattice and ℓ, an integer, for a 'band index'. For clarity, here ℓ singles out one of the (one-dimensional) irreducible representations of the discrete translation group, characterized by $\boldsymbol{k}$. The function $\varphi_{(\boldsymbol{k},\ell);\sigma}(\boldsymbol{r})$ is thus a Bloch function. Now consider the system of *interacting* fermions. From Eqs. (A4) and (A13), and in view of the fact that Eq. (A17) strictly *only* applies to 'non-interacting' systems, we observe that here, in contrast with the 'non-interacting' case, $\{f_{s;\sigma}(\boldsymbol{r})\}$ *cannot* be a basis for some *unitary* irreducible representation of the symmetry group of $u(\boldsymbol{r}) + w_\sigma(\boldsymbol{r})$; note that already the result in Eq. (A20) defies the notion of unitarity. Returning to our above example where $\varsigma = (\boldsymbol{k}, \ell)$, it follows that in general s *cannot* coincide with one particular $(\boldsymbol{k}, \ell)$, but a collection of these, that is all those $(\boldsymbol{k}, \ell)$ associated with non-vanishing contributions to the sum on the RHS of Eq. (A4). In general we have

$$s = \cup_\varsigma\, \varsigma\big|_{\chi_{s;\sigma}(\varsigma)\neq 0}\,. \tag{A21}$$

In words, considering s as a set, it consists of the union of *all* ς (also a *set* of parameters) for which $\chi_{s;\sigma}(\varsigma) \neq 0$ holds; owing to the dependence of $\chi_{s;\sigma}(\varsigma)$ on s, Eq. (A21) amounts to an implicit equation, an intricacy that has its origin in the particle-particle interaction. This repeated incorporation of various elements of the set $\{\varsigma\}$, which is already associated with a *complete* set of basis functions, into the elements of $\{s\}$, implies that the set $\{f_{s;\sigma}(\boldsymbol{r})\}$ must in fact be *over-complete*.

Finally, from the above observations it is evident that "degeneracy" as in "parameter of degeneracy" (Klein and Prange 1958), should be viewed in a somewhat different light than may be implied by the authors (see footnote 50). This is important since, on the one hand, Klein and Prange (1958) deal with $(\boldsymbol{p}, \alpha)$ (*cf.* Eq. (45) above), where $\boldsymbol{p}$ stands for the momentum vector associated with the single-particle excitations of a translational invariant system and α denotes the *"parameter of degeneracy distinguishing states of given momentum"* while, on the other hand, our above discussion makes evident that, even for a translational invariant system (here an attribute of the *GS*, but by no means that of the excited states of such system), $f_{s;\sigma}(\boldsymbol{r})$ is *not* in general capable of being characterized by a *single* momentum, as opposed to a distribution of momenta.

2. Quasi-particles revisited: an approximate treatment

Here we derive a simple expression for the dispersion of the single-particle energies of an interacting uniform system based on an *Ansatz* concerning the $N \pm 1$-particle eigenstates of the interacting Hamiltonian $\widehat{H}$ as presented in Eq. (1). This energy dispersion is determined in terms of the single- and two-particle *static* correlation functions $\Gamma^{(1)}$ and $\Gamma^{(2)}$ pertaining to the GS of this system. As we shall explicitly show, our *Ansatz* with regard to the indicated eigenstates of the system provides an accurate expression for the single-particle excitation energies $\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}$ for $\|\boldsymbol{k} - \boldsymbol{k}_{F;\sigma}\| \to 0$ in the weak-coupling regime. In our general considerations that follow we assume the Hamiltonian to be that pertaining to uniform systems, however, do *not* impose this property on the GS of the system.

Consider the Hamiltonian in Eq. (86). Making use of the expression in Eq. (96), for the GS energy of the corresponding system we have (see Eq. (103))

$$E_{N;0} = e_0\, \bar{E}_{N;0}, \quad \bar{E}_{N;0} = \langle \Psi_{N;0}|\widehat{\mathcal{H}}|\Psi_{N;0}\rangle. \tag{A22}$$

We *assume* the $(N_\sigma \pm 1 + N_{\bar{\sigma}})$-particle eigenstates of the interacting system to be characterized by a single wave-vector $\bar{\boldsymbol{k}}$ (here we consider the case where the change in the number of particles is brought about through a change in that of particles with spin σ); thus we denote these by $|\Psi^0_{N_\sigma\pm 1, N_{\bar{\sigma}};\bar{\boldsymbol{k}}}\rangle$. With

$$\bar{\mu}{:=}\frac{\mu}{e_0} \tag{A23}$$

the normalized 'chemical potential' (see § III.E.1), we have the following for the *single-particle* excitation energies (*cf.* Eq. (19)):

$$\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}{:=}\begin{cases} \bar{E}_{N;0} - \bar{E}_{N_\sigma-1,N_{\bar{\sigma}};\bar{\boldsymbol{k}}}, & \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} < \bar{\mu}, \\ \bar{E}_{N_\sigma+1,N_{\bar{\sigma}};\bar{\boldsymbol{k}}} - \bar{E}_{N;0}, & \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} > \bar{\mu}. \end{cases} \tag{A24}$$

With (see Eq. (A8) above)

$$\nu_\sigma(\bar{\boldsymbol{k}}){:=}\begin{cases} \mathsf{n}_\sigma(\bar{\boldsymbol{k}}/r_0), & \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} < \bar{\mu}, \\ 1-\mathsf{n}_\sigma(\bar{\boldsymbol{k}}/r_0), & \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} > \bar{\mu}, \end{cases} \tag{A25}$$

where $\mathsf{n}_\sigma(\boldsymbol{k})$ denotes the GS momentum distribution function corresponding to spin-σ particles, defined in Eq. (J2), for $\nu_\sigma(\bar{\boldsymbol{k}}) \neq 0$ we make the following *Ansatz* for the $(N_\sigma \mp 1 + N_{\bar{\sigma}})$-particle eigenstates of the interacting system [112]

$$|\Psi^0_{N_\sigma-1,N_{\bar{\sigma}};\bar{\boldsymbol{k}}}\rangle{:=}\frac{1}{\sqrt{\nu_\sigma(\bar{\boldsymbol{k}})}}\,\hat{a}_{\bar{\boldsymbol{k}};\sigma}|\Psi_{N;0}\rangle,\ \ \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} < \bar{\mu}, \tag{A26}$$

$$|\Psi^0_{N_\sigma+1,N_{\bar{\sigma}};\bar{\boldsymbol{k}}}\rangle{:=}\frac{1}{\sqrt{\nu_\sigma(\bar{\boldsymbol{k}})}}\,\hat{a}^\dagger_{\bar{\boldsymbol{k}};\sigma}|\Psi_{N;0}\rangle,\ \ \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} > \bar{\mu}. \tag{A27}$$

It is instructive to examine the properties of these states for the case where the system is non-interacting so that $\nu_\sigma(\bar{\boldsymbol{k}}) = 1$ for $\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} \lessgtr \bar{\mu}$.

It can be readily shown that the states in Eqs. (A26) and (A27) are normalized to unity and, moreover, are eigenstates of the *partial* number operators, in particular of $\widehat{N}_\sigma$ corresponding to eigenvalues $(N_\sigma \mp 1)$ respectively (assuming $N_\sigma \geq 1$).

Following the *Ansätze* in Eqs. (A26) and (A27), for

$$\bar{E}_{N_\sigma\mp1,N_{\bar{\sigma}};\bar{\boldsymbol{k}}}{:=}\langle\Psi^0_{N_\sigma\mp1,N_{\bar{\sigma}};\bar{\boldsymbol{k}}}|\widehat{\mathcal{H}}|\Psi^0_{N_\sigma\mp1,N_{\bar{\sigma}};\bar{\boldsymbol{k}}}\rangle$$

we have

$$\bar{E}_{N_\sigma-1,N_{\bar{\sigma}};\bar{\boldsymbol{k}}} = \frac{1}{\nu_\sigma(\bar{\boldsymbol{k}})}\,\langle\Psi_{N;0}|\hat{a}^\dagger_{\bar{\boldsymbol{k}};\sigma}\widehat{\mathcal{H}}\,\hat{a}_{\bar{\boldsymbol{k}};\sigma}|\Psi_{N;0}\rangle,\quad \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} < \bar{\mu}, \tag{A28}$$

$$\bar{E}_{N_\sigma+1,N_{\bar{\sigma}};\bar{\boldsymbol{k}}} = \frac{1}{\nu_\sigma(\bar{\boldsymbol{k}})}\,\langle\Psi_{N;0}|\hat{a}_{\bar{\boldsymbol{k}};\sigma}\widehat{\mathcal{H}}\,\hat{a}^\dagger_{\bar{\boldsymbol{k}};\sigma}|\Psi_{N;0}\rangle,\quad \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} > \bar{\mu}. \tag{A29}$$

Making use of the identity

$$\widehat{\mathcal{H}}\,\hat{a}_{\bar{\boldsymbol{k}};\sigma} \equiv \big[\widehat{\mathcal{H}},\hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_- + \hat{a}_{\bar{\boldsymbol{k}};\sigma}\,\widehat{\mathcal{H}}, \tag{A30}$$

from Eqs. (A24), (A28) and (A29) we readily deduce that

$$\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} \equiv \begin{cases} -\langle\Psi_{N;0}|\hat{a}^\dagger_{\bar{\boldsymbol{k}};\sigma}\big[\widehat{\mathcal{H}},\hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_-|\Psi_{N;0}\rangle/\nu_\sigma(\bar{\boldsymbol{k}}), \\ \qquad\qquad\qquad\qquad \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} < \bar{\mu}, \\ -\langle\Psi_{N;0}|\big[\widehat{\mathcal{H}},\hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_-\hat{a}^\dagger_{\bar{\boldsymbol{k}};\sigma}|\Psi_{N;0}\rangle/\nu_\sigma(\bar{\boldsymbol{k}}), \\ \qquad\qquad\qquad\qquad \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} > \bar{\mu}. \end{cases} \tag{A31}$$

It is interesting to note that, according to Eq. (A31), $\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}$ is obtained from the knowledge of the GS; in this connection note that $\nu_\sigma(\bar{\boldsymbol{k}})$ is also a GS property (see Eqs. (J2) and (A25)).

From the linearity of $[\,,\,]_-$ we have

$$\big[\widehat{\mathcal{H}},\hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_- = \big[\widehat{\mathcal{T}},\hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_- + \big[\widehat{\mathcal{V}},\hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_-; \tag{A32}$$

in the case of $d=3$ and $v \equiv v_c$, the RHS of Eq. (A32) has to be supplemented by $\big[2\widehat{\mathcal{H}}_{\bar{\kappa}},\hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_-$ where (*cf.* Eq. (5))

$$\widehat{\mathcal{H}}_{\bar{\kappa}}{:=}\frac{1}{e_0}\,\widehat{H}_\kappa \equiv -\bar{\varpi}_{\bar{\kappa}}\,\widehat{N};\quad \bar{\varpi}_{\bar{\kappa}}{:=}\frac{3}{2r_s\,\bar{\kappa}^2},\quad \bar{\kappa}{:=}r_0\kappa. \tag{A33}$$

For the reason underlying the prefactor 2 in $2\widehat{\mathcal{H}}_{\bar{\kappa}}$ see the text following Eq. (9).

Making use of the anticommutation relations in Eq. (101), we readily obtain

$$\big[\widehat{\mathcal{T}},\hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_- = -\frac{1}{2}\,\bar{k}^2\,\hat{a}_{\bar{\boldsymbol{k}};\sigma}, \tag{A34}$$

We point out that, by identifying $\widehat{\mathcal{V}}$ with zero, requiring, in the case of $v \equiv v_c$, identification of $\widehat{\mathcal{H}}_{\bar{\kappa}}$ with zero, from Eqs. (A31) and (A34) we immediately obtain the expected result for the non-interacting single-particle energy dispersion

$$\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} \rightharpoonup \bar{\varepsilon}^{(0)}_{\bar{\boldsymbol{k}}}{:=}\frac{1}{2}\,\bar{k}^2,\quad \bar{\varepsilon}^{(0)}_{\bar{\boldsymbol{k}}} \lessgtr \bar{\mu}. \tag{A35}$$

Thus by writing

$$\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} \equiv \bar{\varepsilon}^{(0)}_{\bar{\boldsymbol{k}}} + \Delta\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}, \tag{A36}$$

the contribution $\Delta\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}$ is obtained from the expression on the RHS of Eq. (A31) through replacing $\widehat{\mathcal{H}}$ herein by $\widehat{\mathcal{V}}$ (by $2\widehat{\mathcal{H}}_{\bar{\kappa}} + \widehat{\mathcal{V}}$ when $v \equiv v_c$) as defined in Eq. (99). Consequently, the *explicit* dependence on r_s of $\Delta\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}$ is linear; as is evident from Eq. (A31), the *implicit* dependence on r_s of this function has its root in the dependences on r_s of $\nu_\sigma(\bar{\boldsymbol{k}})$ and $|\Psi_{N;0}\rangle$. We draw attention to the fact that in view of Eqs. (105) and (A36), $\Delta\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}$ is to be identified with $\overline{\overline{\Sigma}}_\sigma(\bar{\boldsymbol{k}};\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma})$, the on-the-mass-shell SE.

[112] These *Ansätze* are similar in spirit to that by Anderson (1959) (see also Anderson (1987)).

Now we proceed with the determination of the expression for $\Delta\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}$ in terms of practically calculable GS correlation functions. Making use of the expression on the RHS of Eq. (99) and the anticommutation relations in Eq. (101), after some straightforward algebra we obtain [113]

$$\big[\widehat{\mathcal{V}}, \hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_- = \frac{r_s}{\bar{\Omega}} \sum_{\sigma'} \sum_{\bar{\boldsymbol{k}}',\bar{\boldsymbol{q}}'}{}' \bar{w}(\bar{q}')\, \hat{a}^{\dagger}_{\bar{\boldsymbol{k}}'+\bar{\boldsymbol{q}}';\sigma'} \hat{a}_{\bar{\boldsymbol{k}}+\bar{\boldsymbol{q}}';\sigma} \hat{a}_{\bar{\boldsymbol{k}}';\sigma'}. \tag{A37}$$

From this expression, one can directly calculate $\Delta\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}$ corresponding to the case $\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} < \bar{\mu}$ in terms of the two-particle GS correlation function $\Gamma^{(2)}(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2; \boldsymbol{r}_1'\sigma_1', \boldsymbol{r}_2'\sigma_2')$, defined in Appendix B (see Eq. (B8)). In order to obtain a similar expression for $\Delta\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}$ corresponding to the case $\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} > \bar{\mu}$, we need first to bring the pertinent operators into normal order. Making use of Eq. (101) we obtain

$$\begin{aligned}\sum_{\sigma'} \sum_{\bar{\boldsymbol{k}}',\bar{\boldsymbol{q}}'}{}' \bar{w}(\bar{q}')\, \hat{a}^{\dagger}_{\bar{\boldsymbol{k}}'+\bar{\boldsymbol{q}}';\sigma'} \hat{a}_{\bar{\boldsymbol{k}}+\bar{\boldsymbol{q}}';\sigma} \hat{a}_{\bar{\boldsymbol{k}}';\sigma'} \hat{a}^{\dagger}_{\bar{\boldsymbol{k}};\sigma} &= \sum_{\bar{\boldsymbol{q}}'}{}' \bar{w}(\bar{q}')\, \hat{a}^{\dagger}_{\bar{\boldsymbol{k}}+\bar{\boldsymbol{q}}';\sigma} \hat{a}_{\bar{\boldsymbol{k}}+\bar{\boldsymbol{q}}';\sigma} \\ &- \sum_{\sigma'} \sum_{\bar{\boldsymbol{k}}',\bar{\boldsymbol{q}}'}{}' \bar{w}(\bar{q}')\, \hat{a}^{\dagger}_{\bar{\boldsymbol{k}};\sigma} \hat{a}^{\dagger}_{\bar{\boldsymbol{k}}'+\bar{\boldsymbol{q}}';\sigma'} \hat{a}_{\bar{\boldsymbol{k}}+\bar{\boldsymbol{q}}';\sigma} \hat{a}_{\bar{\boldsymbol{k}}';\sigma'}.\end{aligned} \tag{A38}$$

For later use, we present the following expression (see Eq. (A33) above)

$$\big[\widehat{\mathcal{H}}_{\bar{\kappa}}, \hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_- = \bar{\varpi}_{\bar{\kappa}}\, \hat{a}_{\bar{\boldsymbol{k}};\sigma}. \tag{A39}$$

Before casting the expression for $\Delta\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}$ into a form which is suitable for direct (numerical) calculations, we note that the following pairs of Fourier transforms apply

$$\hat{\mathsf{a}}_{\boldsymbol{k};\sigma} = \frac{1}{\Omega^{1/2}} \int_{\Omega} \mathrm{d}^d r\; \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\, \hat{\psi}_{\sigma}(\boldsymbol{r}), \tag{A40}$$

$$\hat{\psi}_{\sigma}(\boldsymbol{r}) = \frac{1}{\Omega^{1/2}} \sum_{\boldsymbol{k}} \mathrm{e}^{+i\boldsymbol{k}\cdot\boldsymbol{r}}\, \hat{\mathsf{a}}_{\boldsymbol{k};\sigma}. \tag{A41}$$

Our use of *summation* over wave-vectors (both here and in the earlier expressions) signifies that we employ a *box* boundary condition; equivalent expressions for the case where wave-vectors are in continuum, are obtained through the substitutions

$$\sum_{\boldsymbol{k}} (\dots) \rightharpoonup \frac{\Omega}{(2\pi)^d} \int \mathrm{d}^d k\, (\dots),\quad \delta_{\boldsymbol{k},\boldsymbol{k}'} \rightharpoonup \frac{(2\pi)^d}{\Omega}\, \delta(\boldsymbol{k}-\boldsymbol{k}'). \tag{A42}$$

Making use of Eq. (A40), we obtain

$$\begin{aligned}\sum_{\sigma'} \langle \Psi_{N;0} | \hat{a}^{\dagger}_{\bar{\boldsymbol{k}};\sigma} \hat{a}^{\dagger}_{\bar{\boldsymbol{k}}'+\bar{\boldsymbol{q}}';\sigma'} \hat{a}_{\bar{\boldsymbol{k}}+\bar{\boldsymbol{q}}';\sigma} \hat{a}_{\bar{\boldsymbol{k}}';\sigma'} | \Psi_{N;0} \rangle &= \frac{-1}{\Omega^2} \int_{\Omega} \Pi_{j=1}^4 \mathrm{d}^d r_j\; \mathrm{e}^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_3)}\, \mathrm{e}^{i\boldsymbol{k}'\cdot(\boldsymbol{r}_2-\boldsymbol{r}_4)}\, \mathrm{e}^{i\boldsymbol{q}'\cdot(\boldsymbol{r}_2-\boldsymbol{r}_3)} \\ &\quad\times \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}_1\sigma, \boldsymbol{r}_2\sigma'; \boldsymbol{r}_3\sigma, \boldsymbol{r}_4\sigma').\end{aligned} \tag{A43}$$

Consequently, through employing (see Eq. (89))

$$w(\|\boldsymbol{r}\|) = \int \frac{\mathrm{d}^d q'}{(2\pi)^d}\; \bar{w}(\|\boldsymbol{q}'\|)\, \mathrm{e}^{i\boldsymbol{q}'\cdot\boldsymbol{r}}, \tag{A44}$$

we arrive at

$$\begin{aligned}\beta^-_{\bar{\boldsymbol{k}};\sigma} &:= \frac{1}{r_s} \langle \Psi_{N;0} | \hat{a}^{\dagger}_{\bar{\boldsymbol{k}};\sigma} \big[\widehat{\mathcal{V}}, \hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_- | \Psi_{N;0} \rangle \\ &= -r_0 \int \mathrm{d}^d r_1\; \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}_1} \int \mathrm{d}^d r_2\; w(\|\boldsymbol{r}_2\|) \\ &\quad\times \sum_{\sigma'} \Gamma^{(2)}\big(\boldsymbol{r}_1\sigma, \boldsymbol{r}_2\sigma'; \boldsymbol{0}\sigma, \boldsymbol{r}_2\sigma'\big),\quad \text{(I)}\end{aligned} \tag{A45}$$

$$\begin{aligned}\beta^-_{\bar{\boldsymbol{k}};\sigma} &:= \frac{1}{r_s} \langle \Psi_{N;0} | \hat{a}^{\dagger}_{\bar{\boldsymbol{k}};\sigma} \big[\widehat{\mathcal{V}} + 2\widehat{\mathcal{H}}_{\bar{\kappa}}, \hat{a}_{\bar{\boldsymbol{k}};\sigma}\big]_- | \Psi_{N;0} \rangle \\ &= -r_0 \int \mathrm{d}^3 r_1\; \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}_1} \int \mathrm{d}^3 r_2\; w_c(\|\boldsymbol{r}_2\|) \\ &\quad\times \sum_{\sigma'} \Big\{ \Gamma^{(2)}\big(\boldsymbol{r}_1\sigma, \boldsymbol{r}_2\sigma'; \boldsymbol{0}\sigma, \boldsymbol{r}_2\sigma'\big) \\ &\qquad - n_{0;\sigma'}\, \varrho_{\sigma}(\boldsymbol{r}_1, \boldsymbol{0}) \Big\},\quad \text{(II)}\end{aligned} \tag{A46}$$

where we have used Eqs. (A37) and (A43) as well as the shift property in Eq. (B14) specific to uniform GSs. For completeness, the expressions in Eqs. (A45) and (A46) have been deduced from ones involving

$$\frac{1}{\Omega} \int \mathrm{d}^d r_3\; \Gamma^{(2)}\big((\boldsymbol{r}_1+\boldsymbol{r}_3)\sigma, (\boldsymbol{r}_2+\boldsymbol{r}_3)\sigma'; \boldsymbol{r}_3\sigma, (\boldsymbol{r}_2+\boldsymbol{r}_3)\sigma'\big),$$

which in consequence of the mentioned shift property together with $\Omega^{-1}\int \mathrm{d}^d r_3 = 1$ has reduced into $\Gamma^{(2)}\big(\boldsymbol{r}_1\sigma, \boldsymbol{r}_2\sigma'; \boldsymbol{0}\sigma, \boldsymbol{r}_2\sigma'\big)$. In Eq. (A45), (I) indicates the case corresponding to short-range interaction potentials, and in Eq. (A46), (II) the case corresponding to $v \equiv v_c$ in $d = 3$.

Making use of Eqs. (A37), (A38) and (A40), in an analogous manner as above, for

[113] Making use of Eqs. (A30), (A34) and (A37) and the fact that $\widehat{\mathcal{H}}|\Psi_{N;0}\rangle = \bar{E}_{N;0}|\Psi_{N;0}\rangle$, one can directly establish the deviation of the states in Eqs. (A26) and (A27) from the true eigenstates of $\widehat{\mathcal{H}}$. This consideration also paves the way for constructing improved states in comparison with those in Eqs. (A26) and (A27).

$$\beta^{+}_{\bar{\boldsymbol{k}};\sigma} := \frac{1}{r_s} \begin{cases} \langle \Psi_{N;0} | \big[\widehat{\mathcal{V}}, \hat{a}_{\bar{\boldsymbol{k}};\sigma} \big]_{-} \hat{a}^{\dagger}_{\bar{\boldsymbol{k}};\sigma} | \Psi_{N;0} \rangle, & \text{(I)} \\ \langle \Psi_{N;0} | \big[\widehat{\mathcal{V}} + 2\widehat{\mathcal{H}}_{\bar{\kappa}}, \hat{a}_{\bar{\boldsymbol{k}};\sigma} \big]_{-} \hat{a}^{\dagger}_{\bar{\boldsymbol{k}};\sigma} | \Psi_{N;0} \rangle & \text{(II)} \end{cases} \tag{A47}$$

we obtain

$$\beta^{+}_{\bar{\boldsymbol{k}};\sigma} = r_0 \int \mathrm{d}^d r_1 \; \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}_1} \, w(\|\boldsymbol{r}_1\|) \, \Gamma^{(1)}\big(\boldsymbol{r}_1\sigma; \boldsymbol{0}\sigma\big) - \beta^{-}_{\bar{\boldsymbol{k}};\sigma}. \tag{A48}$$

In Eq. (A47), (I) and (II) have the same significance as in Eqs. (A45) and (A46). For completeness, we point out that

$$\int \mathrm{d}^d r_1 \; \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}_1} \, w(\|\boldsymbol{r}_1\|) \, \Gamma^{(1)}\big(\boldsymbol{r}_1\sigma; \boldsymbol{0}\sigma\big) \equiv \int \frac{\mathrm{d}^d q'}{(2\pi)^d} \; \bar{w}(q') \, \mathsf{n}_\sigma(\boldsymbol{k} + \boldsymbol{q}'). \tag{A49}$$

Since (unless $\mathsf{n}_\sigma(\boldsymbol{k}) \equiv 0$, corresponding to a GS with *no* particles of spin σ, i.e. $N_\sigma = 0$), $\mathsf{n}_\sigma(\boldsymbol{k})$ is positive, from Eq. (A49) and the assumption that $\bar{w}(q') \geq 0$ for all q' (a non-attractive interaction potential), it follows that the first term on the RHS of Eq. (A48) is in general positive definite.

Combining the above results, from Eq. (A36) we obtain

$$\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} = \bar{\varepsilon}^{(0)}_{\bar{\boldsymbol{k}}} - r_s \, \frac{\beta^{\mp}_{\bar{\boldsymbol{k}};\sigma}}{\nu_\sigma(\bar{\boldsymbol{k}})}, \;\; \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} \lessgtr \bar{\mu}. \tag{A50}$$

Note how effects of interaction on the single-particle excitation energies are accounted for by this expression; in particular the occurrence of $\nu_\sigma(\bar{\boldsymbol{k}})$ in denominator clearly indicates the non-perturbative nature of this expression. On the other hand, since according to the expression in Eq. (A50), the single-particle excitation energy is a well-defined real-valued quantity for *all* $\bar{\boldsymbol{k}}$, this expression should be necessarily of limited validity; as we have discussed in § III.D, the equation for the single-particle excitation energies (see Eq. (105)) does *not* have any (real-valued) solution in regions along the $\bar{\varepsilon}$ axis where $\mathrm{Im}[\overline{\overline{\Sigma}}_\sigma(\bar{\boldsymbol{k}};\bar{\varepsilon})] \not\equiv 0$; real-valued $\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}$ for *all* $\bar{\boldsymbol{k}}$ is only possible when $\mathrm{Im}[\overline{\overline{\Sigma}}_\sigma(\bar{\boldsymbol{k}};\bar{\varepsilon})] \equiv 0$, $\forall \varepsilon$, which is *exclusively* the case for non-interacting systems, or within mean-field frameworks. [114] On the other hand, since $\mathrm{Im}[\overline{\overline{\Sigma}}_\sigma(\bar{\boldsymbol{k}};\bar{\varepsilon}_F)] \equiv 0$, $\forall \bar{\boldsymbol{k}}$ (Galitskii and Migdal 1958, Luttinger 1960, equations (6) and (94)), it is *not* possible *a priori* to decide on the possible inaccuracy of the expression in Eq. (A50) for $\|\bar{\boldsymbol{k}} - \bar{\boldsymbol{k}}_{F;\sigma}\| \to 0$ on the grounds that it is real valued for *all* $\bar{\boldsymbol{k}}$. Later in this Section we demonstrate that $\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}$ in Eq. (A50) coincides to at least linear order in r_s with the expected energy dispersion in the weak-coupling regime. This implies that, through substitution of $\bar{\varepsilon}_{\bar{k};\sigma}$ on both sides of Eq. (146) by the expression on the RHS of Eq. (A50), one can solve for $\beta^{\mp}_{\bar{k};\sigma}$ in the weak-coupling regime and thus bypass the direct evaluation of $\beta^{\mp}_{\bar{k};\sigma}$ according to the expressions in Eqs. (A45), (A46) and (A48).

For *metals* we must have

$$\lim_{\bar{\boldsymbol{k}} \to \bar{\boldsymbol{k}}_{F;\sigma} - \boldsymbol{0}^+} \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} = \lim_{\bar{\boldsymbol{k}} \to \bar{\boldsymbol{k}}_{F;\sigma} + \boldsymbol{0}^+} \bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma}, \tag{A51}$$

which through Eq. (A50) implies

$$\frac{\beta^{-}_{\bar{\boldsymbol{k}};\sigma}}{\nu_\sigma(\bar{\boldsymbol{k}} - \boldsymbol{0}^+)} = \frac{\beta^{+}_{\bar{\boldsymbol{k}};\sigma}}{\nu_\sigma(\bar{\boldsymbol{k}} + \boldsymbol{0}^+)}, \;\; \text{for } \bar{\boldsymbol{k}} = \bar{\boldsymbol{k}}_{F;\sigma}; \tag{A52}$$

our use of $\pm\boldsymbol{0}^+$ here is dictated by the fact that $\mathsf{n}_\sigma(\bar{\boldsymbol{k}}/r_0)$, and thus $\nu_\sigma(\bar{\boldsymbol{k}})$ (see Eq. (A25)), is non-analytic at $\bar{\boldsymbol{k}} = \bar{\boldsymbol{k}}_{F;\sigma}$; for metallic GSs corresponding to continuously differentiable $\overline{\overline{\Sigma}}_\sigma(\bar{k}_{F;\sigma};\bar{\varepsilon})$ with respect to $\bar{\varepsilon}$ in a neighbourhood of $\bar{\varepsilon} = \bar{\varepsilon}_F$, $\mathsf{n}_\sigma(\bar{k}/r_0)$ is *discontinuous* at $\bar{k} = \bar{k}_{F;\sigma}$ (Farid 1999c). Note that, since $\bar{\varepsilon}_F$ is *independent* of σ, Eqs. (A51) and (A52) still apply on replacing σ on their RHSs by $\sigma' \neq \sigma$ so long as $N_{\sigma'} \geq 1$ (see footnote 87). With reference to our considerations in §§ III.E.5,6, on account of the Seitz (1940, pp. 343 and 344) theorem, within the framework of our *Ansatz* for (see footnote 78)

[114] We should emphasize that here the real-valuedness of the single-particle excitation energies $\varepsilon_{s;\sigma}$ as defined in Eq. (19) is *not* at issue; at issue is the real-valuedness of $\varepsilon_{\boldsymbol{k};\sigma}$, characterized solely by $\boldsymbol{k}$ rather than $s = (\boldsymbol{k}, \alpha)$, with α the "parameter of degeneracy" introduced and discussed in § III.B (see Eq. (45)). In this context, one can think of a generalization of the *Ansätze* in Eqs. (A26) and (A27) according to which the pertinent states are characterized not only by $\boldsymbol{k}$ but also by a set of additional parameters that render the employed $(N_\sigma \pm 1 + N_{\bar{\sigma}})$-particle states better variational eigenstates of the interacting Hamiltonian than those presented in Eqs. (A26) and (A27). These additional parameters bring about the possibility that, for a given $\boldsymbol{k}$, the optimal parameters are *not* unique, that is a multiplicity of different values for these parameters give rise to variational states corresponding to different $(N_\sigma \pm 1 + N_{\bar{\sigma}})$-particle eigenstates of the interacting Hamiltonian. In consequence of this mechanism, on taking full or sufficiently detailed account of α, one establishes that to a given $\boldsymbol{k}$ corresponds not one eigenstate, but a continuous *distribution* of eigenstates whose corresponding energies, as measured with respect to the energy of the $(N_\sigma + N_{\bar{\sigma}})$-particle GS of the interacting Hamiltonian, show up as peaks of finite widths in the depiction of the single-particle spectral function $A_\sigma(\boldsymbol{k};\varepsilon)$ along the ε axis, which naturally are *not* capable of being described in terms of real-valued energies $\varepsilon_{\boldsymbol{k};\sigma}$.

$$\bar{\mu}_{\rm xc} := \frac{{\rm d}[n\bar{E}_{\rm xc}(n)]}{{\rm d}n} \equiv (\bar{\varepsilon}_{\bar{\boldsymbol{k}};\sigma} - \bar{\varepsilon}^{(0)}_{\bar{\boldsymbol{k}}})\Big|_{\bar{\boldsymbol{k}}=\bar{\boldsymbol{k}}_{F;\sigma}} \equiv \bar{\varepsilon}_F - \bar{\varepsilon}_F^{(0)}, \qquad (A53)$$

we have

$$\bar{\mu}_{\rm xc} = \frac{-r_s\, \beta^{\mp}_{\bar{\boldsymbol{k}};\sigma}}{\nu_\sigma(\bar{\boldsymbol{k}} \mp \boldsymbol{0}^+)}\Bigg|_{\bar{\boldsymbol{k}}=\bar{\boldsymbol{k}}_{F;\sigma}}, \quad \forall\,\sigma \;\text{ with }\; N_\sigma \neq 0. \qquad (A54)$$

This expression can serve as a basis for determining the accuracy of the *Ansätze* from which it is deduced, by comparing $\bar{\mu}_{\rm xc}$ (for some finite range of r_s values) as calculated according to Eq. (A54) with that deduced from the total energy pertaining to the correlated N-particle GS $|\Psi_{N;0}\rangle$ in Eqs. (A26) and (A27) (for details see footnote 78).

In the remaining part of this Section we specialize to systems with uniform *and* isotropic metallic GSs. We further assume that the Fermi sea pertaining to particles with spin σ is simply connected so that it is characterized by a single Fermi wavenumber $\bar{k}_{F;\sigma}$.

Within the SSDA, where

$$\sum_{\sigma'} \Big\{ \Gamma^{(2)}(\boldsymbol{r}_1\sigma, \boldsymbol{r}_2\sigma'; \boldsymbol{0}\sigma, \boldsymbol{r}_2\sigma') - n_{0;\sigma'}\, \varrho_\sigma(\boldsymbol{r}_1, \boldsymbol{0}) \Big\}\Bigg|_{\rm s} = -\varrho^{\rm h}_{{\rm s};\sigma}(\|\boldsymbol{r}_2\|)\, \varrho^{\rm h}_{{\rm s};\sigma}(\|\boldsymbol{r}_1 - \boldsymbol{r}_2\|), \qquad (A55)$$

from Eq. (A46) for $v \equiv v_c$ in $d = 3$ we readily obtain

$$\beta^{-}_{\bar{k};\sigma}\Big|_{\rm s} = \frac{2}{\pi}\, \bar{k}_{F;\sigma} {\sf F}(\bar{k}/\bar{k}_{F;\sigma})\, {\sf n}_{{\rm s};\sigma}(\bar{k}), \qquad (A56)$$

where ${\sf F}(x)$ is defined in Eq. (131) and

$${\sf n}_{{\rm s};\sigma}(\bar{k}) \equiv \Theta(\bar{k}_{F;\sigma} - \bar{k}) \qquad (A57)$$

is the GS momentum distribution function pertaining to the system of non-interacting fermions. In obtaining the result in Eq. (A56) we have made use of the expression for $\varrho^{\rm h}_{{\rm s};\sigma}(\|\boldsymbol{r}\|)$ as presented in Eq. (F24). With (*cf.* Eq. (B16)) [115]

$$r_0 \int {\rm d}^3 r_1\; {\rm e}^{i\boldsymbol{k}\cdot\boldsymbol{r}_1}\, w_c(\|\boldsymbol{r}_1\|)\, \Gamma^{(1)}_{\rm s}(\boldsymbol{r}_1\sigma; \boldsymbol{0}\sigma) = \frac{2}{\pi}\, \bar{k}_{F;\sigma} {\sf F}(\bar{k}/\bar{k}_{F;\sigma}), \qquad (A58)$$

from Eqs. (A48) and (A56) we obtain

$$\beta^{+}_{\bar{k};\sigma}\Big|_{\rm s} = \frac{2}{\pi} \bar{k}_{F;\sigma} {\sf F}(\bar{k}/\bar{k}_{F;\sigma})\, \big(1 - {\sf n}_{{\rm s};\sigma}(\bar{k})\big). \qquad (A59)$$

From Eqs. (A50), (A56) and (A59) we thus have

$$\bar{\varepsilon}_{\bar{k};\sigma}\big|_{\rm s} = \bar{\varepsilon}^{(0)}_{\bar{k}} - \frac{2}{\pi}\, \bar{k}_{F;\sigma}\, r_s\, {\sf F}(\bar{k}/\bar{k}_{F;\sigma}), \qquad (A60)$$

which for systems of spin-1/2 fermions in the paramagnetic state, for which $\bar{k}_{F;\sigma} \equiv \bar{k}_F = (9\pi/4)^{1/3} \approx 1.919$, exactly reproduces the conventional Hartree-Fock result for the single-particle excitation energies (see footnote 75). It follows that the expression in Eq. (A50) is exact to at least the linear order in r_s in the weak-coupling regime. In the light of our considerations subsequent to Eq. (A50) above, the latter observation is mainly of significance for $\|\bar{\boldsymbol{k}} - \bar{\boldsymbol{k}}_{F;\sigma}\| \to 0$.

Now we proceed by assuming that in addition to being uniform and isotropic, the GS of the system is also a Fermi-liquid metallic state. Consequently (for example Farid (1999c)), in a neighbourhood of $k_{F;\sigma}$, we have the following relation (unless stated otherwise, below energies and momenta are *not* normalized)

$$\varepsilon_{k;\sigma} = \varepsilon_F + \hbar v_{F;\sigma}(k - k_{F;\sigma}) + o(k - k_{F;\sigma}), \qquad (A61)$$

where

$$v_{F;\sigma} := \frac{1}{\hbar}\, \frac{{\rm d}\varepsilon_{k;\sigma}}{{\rm d}k}\Big|_{k=k_{F;\sigma}} \equiv \frac{\hbar k_{F;\sigma}}{m^\star_\sigma} \qquad (A62)$$

is the Fermi velocity in terms of which the effective mass $m^\star_\sigma$ for quasi-particles with spin index σ is defined. From the quasi-particle equation in Eq. (105) we have, however, [116]

$$\frac{1}{\hbar}\, \frac{{\rm d}\varepsilon_{k;\sigma}}{{\rm d}k}\Big|_{k=k_{F;\sigma}} = Z_{F;\sigma} \Big\{ v^{(0)}_{F;\sigma} + \frac{{\rm d}\overline{\Sigma}_\sigma(k;\varepsilon_F)}{{\rm d}k}\Big|_{k=k_{F;\sigma}} \Big\}, \qquad (A63)$$

where $v^{(0)}_{F;\sigma} := \hbar^{-1} {\rm d}\varepsilon^{(0)}_k/{\rm d}k|_{k=k_{F;\sigma}}$ denotes the Fermi velocity of the non-interacting particles (note that the dependence on σ of $v^{(0)}_{F;\sigma}$ is entirely due to that of $k_{F;\sigma}$ on σ). With the amount of the jump $Z_{F;\sigma}$ in the momentum-distribution function ${\sf n}_\sigma(k)$ (see Eq. (J7)) at $k = k_{F;\sigma}$ being determined from

$$Z_{F;\sigma} = \Big(1 - \hbar\, \frac{{\rm d}\overline{\Sigma}_\sigma(k_{F;\sigma};\varepsilon)}{{\rm d}\varepsilon}\Big|_{\varepsilon=\varepsilon_F}\Big)^{-1}, \qquad (A64)$$

we observe that the knowledge of $Z_{F;\sigma}$, $v_{F;\sigma}$ (or $m^\star_\sigma$) and ε_F is sufficient to describe fully the leading-order asymptotic behaviour of $\overline{\Sigma}_\sigma(k;\varepsilon)$ corresponding to a Fermi-liquid metallic state for $k \to k_{F;\sigma}$ and $\varepsilon \to \varepsilon_F$. This

[115] Here we have $\Gamma^{(1)}_{\rm s}(\boldsymbol{r}_1\sigma; \boldsymbol{0}\sigma) \equiv \varrho^{\rm h}_{{\rm s};\sigma}(\|\boldsymbol{r}_1\|)$ (see Eqs. (B16) and (F9)). Consequently, the result in Eq. (A58) is relevant to that in Eq. (130).

[116] Below $\overline{\Sigma}(k;\varepsilon)$ denotes the Fourier representation of the SE operator and *not* the normalized SE as in Eq. (104).

follows from the fact that $\overline{\Sigma}_\sigma(k;\varepsilon)$ pertaining to a Fermi-liquid metallic state is uniquely characterized by the following two properties (Farid 1999c).

(A) $\overline{\Sigma}_\sigma(k_{F;\sigma};\varepsilon)$ is continuously differentiable with respect to ε in a neighbourhood of $\varepsilon = \varepsilon_F$.

(B) $\overline{\Sigma}_\sigma(k;\varepsilon_F)$ is continuously differentiable with respect to k in a neighbourhood of $k = k_{F;\sigma}$.

Consequently (and this constitutes the foundation of Eq. (A61) above), for $\widetilde{\overline{\Sigma}}_\sigma(k;z)$ pertaining to a Fermi-liquid metallic state we can write

$$\widetilde{\overline{\Sigma}}_\sigma(k;z) = (\varepsilon_F - \varepsilon_{F;\sigma}^{(0)}) + \mathsf{A}_\sigma(k - k_{F;\sigma}) + \mathsf{B}_\sigma(z - \varepsilon_F) + o(k - k_{F;\sigma}) + o(z - \varepsilon_F), \qquad \text{(A65)}$$

where $\varepsilon_{F;\sigma}^{(0)} := \varepsilon_k^{(0)}|_{k=k_{F;\sigma}}$,

$$\mathsf{A}_\sigma := \left.\frac{\mathrm{d}\overline{\Sigma}_\sigma(k;\varepsilon_F)}{\mathrm{d}k}\right|_{k=k_{F;\sigma}} \equiv \frac{v_{F;\sigma}}{Z_{F;\sigma}} - v_{F;\sigma}^{(0)}, \qquad \text{(A66)}$$

$$\mathsf{B}_\sigma := \left.\frac{\mathrm{d}\overline{\Sigma}_\sigma(k_{F;\sigma};\varepsilon)}{\mathrm{d}\varepsilon}\right|_{\varepsilon=\varepsilon_F} \equiv \frac{1}{\hbar}\Big(1 - \frac{1}{Z_{F;\sigma}}\Big). \qquad \text{(A67)}$$

We point out that, to the order in which $\widetilde{\overline{\Sigma}}_\sigma(k;z)$ is presented in Eq. (A65), it is real-valued for z identified with a real-valued energy parameter ε. The first term on the RHS of Eq. (A65) can be directly determined from the expression in Eq. (A50); it can also be determined from knowledge of the total energy of the interacting system as function of the constant particle density n_0 through application of the Seitz (1940, pp. 343 and 344) theorem (see Eqs. (A53) and (A54); see also footnote 78). As is evident from Eqs. (A48) and (A49), calculation of $\beta^{+}_{\boldsymbol{k};\sigma}$ requires knowledge of $\mathsf{n}_\sigma(\boldsymbol{k})$ from which $Z_{F;\sigma}$ is deduced, through $Z_{F;\sigma} = \mathsf{n}_\sigma(k_{F;\sigma} - 0^+) - \mathsf{n}_\sigma(k_{F;\sigma} + 0^+)$ (Migdal 1957, Luttinger 1960) (see Eq. (J7)). With the knowledge of $Z_{F;\sigma}$ and $v_{F;\sigma}$ (or $m^\star_\sigma$; see Eq. (A62) above), A_σ is readily obtained through employing the expression in Eq. (A66); B_σ, on the other hand, is fully determined by $Z_{F;\sigma}$.

In § IV.D we present a *constrained* interpolation of the SE operator $\Sigma_\sigma(\varepsilon)$, interpolating between the first-order term of the perturbation series of this operator in terms of the dynamically-screened particle-particle interaction functions W for ε close to the 'chemical potential' μ, and the exact asymptotic expression (as described in terms of a finite number of leading-order terms of the large-$|\varepsilon|$ AS for $\Sigma_\sigma(\varepsilon)$) for 'large' values of $|\varepsilon|$. Although the constraints imposed on the global behaviour of the mentioned interpolation expression, which we in § IV.D denote by $\mathsf{f}_{\mathrm{m}}^{(1)}(\varepsilon)$, necessarily bring about change in the behaviour of the interpolated $\Sigma_\sigma(\varepsilon)$ for ε close to μ, in comparison with that of the first-order approximation to the SE operator (for one such constraint see the next paragraph), such change is *not* explicitly controlled. This limitation can be removed by means of extending the scheme in § IV.D in such a way that it admits *direct* adjustment for ε in the vicinity of μ and imposing the expected behaviour on the interpolating function in this regime. In this context, the expression in Eq. (A65), combined with the large-$|z|$ asymptotic expressions for $\widetilde{\overline{\Sigma}}_\sigma(k;z)$ in Eqs. (128) and (129), is of particular relevance to uniform and isotropic metallic states that can be classified as Fermi liquids.

With reference to an observation by Kajueter and Kotliar (1996) in their treatment of the Anderson impurity model, we point out that imposition of the Luttinger-Ward (1960) *identity* [117]

$$\int_{\mu-i\infty}^{\mu+i\infty} \mathrm{d}z\; \widetilde{G}_\sigma(z)\, \frac{\mathrm{d}\widetilde{\Sigma}_\sigma(z)}{\mathrm{d}z} \equiv -\int_{\mu-i\infty}^{\mu+i\infty} \mathrm{d}z\; \widetilde{\Sigma}_\sigma(z)\, \frac{\mathrm{d}\widetilde{G}_\sigma(z)}{\mathrm{d}z} \equiv 0 \qquad \text{(A68)}$$

on an approximate expression for $\widetilde{\overline{\Sigma}}_\sigma(k;z)$ can considerably enhance the accuracy of the approximation. For completeness we note that inspection of the work by Luttinger and Ward (1960) (see specifically the text following Eq. (36) in the latter work) reveals that the identity in Eq. (A68) is a direct manifestation of the conservation of energy at the interaction vertices of the diagrammatic representations of $\widetilde{G}_\sigma(z)$ and $\widetilde{\Sigma}_\sigma(z)$. Thus Eq. (A68) amounts to an identity not only for the *exact* $\widetilde{G}_\sigma(z)$ and $\widetilde{\Sigma}_\sigma(z)$, but also for approximate $\widetilde{\Sigma}_\sigma(z)$ and $\widetilde{G}_\sigma(z)$ that in particular are calculated within the framework of the many-body perturbation theory; Eq. (A68) may however

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[117] See Eq. (63) in the paper by Luttinger and Ward (1960). See also Eqs. (12) and (13) in the paper by Langer and Ambegaokar (1961) and Eq. (51) in the paper by Farid (1999a); the expressions in the latter two works are less restrictive than the expression in the original work by Luttinger and Ward (1960) which pertains to uniform and isotropic systems and moreover involves a trace over momenta. A careful analysis of the details underlying the work by the latter workers reveals that these restrictions are *not* essential. We note in passing that the two expressions in Eq. (68) are *not* independent; one is obtained from the other through integration by parts, which in consequence of the expressions in Eqs. (61) and (72) does *not* lead to finite contributions corresponding to the end-points of the integration interval. For completeness, let $\tilde{f}_\sigma(z) := \widetilde{G}_\sigma(z)\mathrm{d}\widetilde{\Sigma}_\sigma(z)/\mathrm{d}z$ and $\tilde{g}_\sigma(z) := \widetilde{\Sigma}_\sigma(z)\mathrm{d}\widetilde{G}_\sigma(z)/\mathrm{d}z$. With (see Eqs. (25), (65), (26) and (67) and compare with Eq. (39)) $\mathsf{f}_\sigma(\varepsilon) := \lim_{\eta\downarrow 0}[\tilde{f}_\sigma(\varepsilon - i\eta) - \tilde{f}_\sigma(\varepsilon + i\eta)]/(2\pi i)$ and $\mathsf{g}_\sigma(\varepsilon) := \lim_{\eta\downarrow 0}[\tilde{g}_\sigma(\varepsilon - i\eta) - \tilde{g}_\sigma(\varepsilon + i\eta)]/(2\pi i)$, Eq. (A68) can be shown to be equivalent to $\int_{-\infty}^{\mu} \mathrm{d}\varepsilon\; \mathsf{f}_\sigma(\varepsilon) \equiv -\int_{-\infty}^{\mu} \mathrm{d}\varepsilon\; \mathsf{g}_\sigma(\varepsilon) \equiv 0$.

be violated when the expressions for $\widetilde{\Sigma}_\sigma(z)$ and $\widetilde{G}_\sigma(z)$ are postulated. Consequently, only in these cases can Eq. (68) amount to a nontrivial condition.

Finally, consider (*cf.* Eq. (A62) above)

$$\bar{v}_{\bar{k};\sigma} := \frac{\mathrm{d}\bar{\varepsilon}_{\bar{k};\sigma}}{\mathrm{d}\bar{k}}. \tag{A69}$$

From the expression in Eq. (A50) we obtain

$$\bar{v}_{\bar{k};\sigma} = \bar{v}_{\bar{k}}^{(0)} - \frac{r_s}{\nu_\sigma(\bar{k})} \times \Big(\frac{\mathrm{d}}{\mathrm{d}\bar{k}}\, \beta^{\mp}_{\bar{k};\sigma} - \beta^{\mp}_{\bar{k};\sigma} \frac{\mathrm{d}}{\mathrm{d}\bar{k}} \ln\big(\nu_\sigma(\bar{k})\big)\Big), \;\; \bar{k} \lessgtr \bar{k}_{F;\sigma}, \tag{A70}$$

where $\bar{v}_{\bar{k}}^{(0)} := \mathrm{d}\bar{\varepsilon}_{\bar{k}}^{(0)}/\mathrm{d}\bar{k}$. The expression in Eq. (A70) is of interest to us particularly for $\bar{k} \uparrow \bar{k}_{F;\sigma}$ and $\bar{k} \downarrow \bar{k}_{F;\sigma}$. With reference to Eq. (A25), from this, one would expect that divergent derivatives with respect to $\bar{k}$ of $\beta^{\mp}_{\bar{k};\sigma}$ and $\nu_\sigma(\bar{k})$ to the left and right of $\bar{k}_{F;\sigma}$ respectively would necessarily imply a vanishing $m^\star_\sigma$ (see Eq. (A62) above) and consequently breakdown of Fermi-liquid metallic state. As we have discussed in (Farid 1999c), [118] for Fermi liquids $\mathrm{d}\mathsf{n}_\sigma(\bar{k})/\mathrm{d}\bar{k}$ can in principle diverge for $\bar{k} \uparrow \bar{k}_{F;\sigma}$. In fact, for a uniform and isotropic system of fermions interacting through a short-range potential, Belyakov (1961) (see also Sartor and Mahaux (1980)) calculated the GS $\mathsf{n}_\sigma(\bar{k})$ of which the left and the right derivatives with respect to $\bar{k}$ are logarithmically divergent at $\bar{k}_{F;\sigma}$ (see Eq. (J9) and the subsequent text). It is seen from Eq. (A70) that *cancellation* of the possible divergent contributions to the terms enclosed by the large parentheses allows for a *finite* renormalization of $\bar{v}_{F;\sigma}$ with respect to $\bar{v}_{F;\sigma}^{(0)}$, or a non-vanishing $m^\star_\sigma$, in spite of the possible divergence of $\mathrm{d}\mathsf{n}_\sigma(\bar{k})/\mathrm{d}\bar{k}$ to the left and/or to the right of $\bar{k} = \bar{k}_{F;\sigma}$ (see Appendix J, in particular the last paragraph herein).

From Eq. (A70) we further observe the possibility that $\bar{v}_{\bar{k};\sigma}$ *may* vanish for $\bar{k} = \bar{k}_{F;\sigma}$, implying, according to Eq. (A62), a divergent $m^\star_\sigma$. This possibility is *not*, however, directly tied with the condition $Z_{F;\sigma} \to 0$, where $Z_{F;\sigma}$ denotes the amount of jump in $\mathsf{n}_\sigma(\bar{k})$ at $\bar{k} = \bar{k}_{F;\sigma}$. This is in contrast with the expected behaviour according to the Gutzwiller (1963, 1964, 1965) *Ansatz* for the GS wavefunction of the Hubbard Hamiltonian in conjunction with the Gutzwiller *approximation* (for example Gebhard (1997, § 3.4)), where $m^\star/m_e = 1/Z_F$ (see Brinkman and Rice (1970b, Eq. (7)) and note that Brinkman and Rice denote Z_F by q). For completeness, we mention that in the considerations by Brinkman and Rice (1970b) the contribution to the effective mass due to the momentum dependence of the SE has *not* been taken into account; this amounts to neglect of the second term enclosed by large parentheses on the RHS of Eq. (A63). We emphasize that the expression in Eq. (A50), and thus that in Eq. (A70), does *not* involve any approximation associated with the correlated GS of the N-particle system so that $\Gamma^{(1)}$ and $\Gamma^{(2)}$ which determine $\beta^{\mp}_{\bar{k};\sigma}$ (see Eqs. (A45), (A46) and (A48)) are the *exact* GS correlations functions. Consequently, the approximate nature of the energy expression in Eq. (A50) is *wholly* attributable to our assumptions in Eqs. (A26) and (A27) concerning the ground and excited states of the $(N_\sigma \mp 1 + N_{\bar{\sigma}})$-particle system. In the considerations by Brinkman and Rice (1970b), on the other hand, the underlying approximation (aside from that, which is unimportant in the present context, just mentioned above) concerns the GS of the N-particle system under consideration, taken to be the Gutzwiller (1963, 1964, 1965) *Ansatz* and dealt with according to the Gutzwiller (1963, 1964, 1965) *approximation*.

□

[118] See the paragraph preceding that containing Eq. (33) in the paper by Farid (1999c).

APPENDIX B: ON THE DENSITY MATRICES $\Gamma^{(m)}$ AND THEIR ASSOCIATION WITH $n_\sigma(\boldsymbol{r})$, $\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}')$ AND $\mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}')$

Here we introduce a hierarchy of *static* correlation functions, denoted by $\Gamma^{(m)}(x_1,\dots,x_m;x_1',\dots,x_m')$, $0 \le m \le N$, with $x_i \equiv \boldsymbol{r}_i\sigma_i$, pertaining to the N-particle GSs of interacting systems of spin-s fermions described by the many-body Hamiltonian $\widehat{H}$ in Eq. (1). These functions are defined as the GS expectation values of the normal-ordered products of m *pairs* of creation and annihilation field operators in the Schrödinger picture (for this and other 'pictures', see, for example Fetter and Walecka (1971, pp. 53-59)). In this Appendix we deduce the expression for $\Gamma^{(m)}$ in terms of a configuration-space integral of the GS wavefunction. These expressions are specifically useful for the purpose of numerical calculations; in these calculations, under the condition $N - m \gtrsim 4$, the mentioned configuration-space integrals are most efficiently evaluated by means of the Monte Carlo importance sampling technique (Negele and Orland 1988, chapter 8).

Since the first-quantized counterpart of $\widehat{H}$ in Eq. (1) is real, unless otherwise stated or implied, in the following as well as in other parts of this work we assume the coordinate representation of the N-particle GS of $\widehat{H}$ to be real-valued; with this assumption we fix the global gauge of the problem at hand, that is, once the zero of the external potential $u(\boldsymbol{r})$ in Eq. (2) has been fixed, it is no longer permitted to subject $u(\boldsymbol{r})$ to a constant (i.e. *global*) arbitrary shift, which otherwise is of no consequence to observable quantities. We further assume the GS of $\widehat{H}$ to be *normal* and *non*-degenerate.

We define (for example March, *et al.* (1967 chapter 1))

$$\Gamma^{(m)}(\boldsymbol{r}_1\sigma_1,\dots,\boldsymbol{r}_m\sigma_m;\boldsymbol{r}'_1\sigma'_1,\dots,\boldsymbol{r}'_m\sigma'_m) := \langle\Psi_{N;0}|\hat{\psi}^{\dagger}_{\sigma_1}(\boldsymbol{r}_1)\dots\hat{\psi}^{\dagger}_{\sigma_m}(\boldsymbol{r}_m) \times\hat{\psi}_{\sigma'_m}(\boldsymbol{r}'_m)\dots\hat{\psi}_{\sigma'_1}(\boldsymbol{r}'_1)|\Psi_{N;0}\rangle. \quad \text{(B1)}$$

Orthogonality of N-particle states corresponding to different N_σ, $\forall\sigma$, or, what is the same, conservation of spin implies that

$$\Gamma^{(m)}(\boldsymbol{r}_1\sigma_1,\dots,\boldsymbol{r}_m\sigma_m;\boldsymbol{r}'_1\sigma'_1,\dots,\boldsymbol{r}'_m\sigma'_m) \equiv 0, \quad \neg\exists\,\mathcal{P}^{(m)} \text{ for which } \sigma_i = \sigma'_{\mathcal{P}^{(m)}i},\ \forall i, \quad \text{(B2)}$$

where $\mathcal{P}^{(m)}i$ stands for a permutation of i over the set $\{1,\dots,m\}$.

The prescription with regard to the coordinate representation of the $(N-1)$-particle state resulting from the operation of $\hat{\psi}_\sigma(\boldsymbol{r}) \equiv \hat{\psi}(x)$, with $x \equiv \boldsymbol{r}\sigma$, on an N-particle state, such as $|\Psi_{N;0}\rangle$ whose coordinate representation we denote by $\Psi_{N;0}(x_1,\dots,x_N)$, is as follows (for example McWeeny 1992, pp. 460-464):

$$\hat{\psi}(x)|\Psi_{N;0}\rangle \rightharpoonup N^{1/2}\Psi_{N;0}(x_1,\dots,x_{N-1},x), \quad \text{(B3)}$$

that is, the coordinate representation of the state corresponding to $\hat{\psi}(x)|\Psi_{N;0}\rangle$ is equal to $N^{1/2}$ times the coordinate representation of $|\Psi_{N;0}\rangle$ in which the Nth spin-orbit coordinate x_N has been replaced by $x \equiv \boldsymbol{r}\sigma$; the state thus obtained, is an $(N-1)$-particle state (it is, however, not an eigenstate [119] of $\widehat{H}$ nor is it normalized to unity) in which x plays the role of an *external* parameter. From Eq. (B3) and the fact that $\hat{\psi}(x)|\Psi_{N;0}\rangle$ is an $(N-1)$-particle state, it follows that

$$\hat{\psi}(x')\,\hat{\psi}(x)|\Psi_{N;0}\rangle \rightharpoonup (N-1)^{1/2}N^{1/2} \times\Psi_{N;0}(x_1,\dots,x_{N-2},x',x). \quad \text{(B4)}$$

Since $\hat{\psi}^{\dagger}(x) \equiv \hat{\psi}^{\dagger}_{\sigma}(\boldsymbol{r})$ is the Hermitian conjugate of $\hat{\psi}(x)$, from Eq. (B3) we readily obtain

$$\langle\Psi_{N;0}|\hat{\psi}^{\dagger}(x) \rightharpoonup N^{1/2}\Psi^*_{N;0}(x_1,\dots,x_{N-1},x), \quad \text{(B5)}$$

and similarly, from Eq. (B4),

$$\langle\Psi_{N;0}|\hat{\psi}^{\dagger}(x)\,\hat{\psi}^{\dagger}(x') \rightharpoonup (N-1)^{1/2}N^{1/2} \times\Psi^*_{N;0}(x_1,\dots,x_{N-2},x',x). \quad \text{(B6)}$$

The results in Eqs. (B3) and (B4) can be easily generalized for products of an arbitrary number of field operators, taking into account however that

$$\hat{\psi}(x_M)\hat{\psi}(x_{M-1})\dots\hat{\psi}(x_1)|\Psi_{N_\sigma,N_{\bar{\sigma}};0}\rangle \equiv 0 \quad \text{when} \quad \sum_{i=1}^{M}\delta_{\sigma_i,\sigma} > N_\sigma,\ \forall\sigma, \quad \text{(B7)}$$

which reflects the fact that the partial number operators $\{\widehat{N}_\sigma\}$ are positive *semi*-definite.

From the above prescriptions and Eq. (B1) we immediately obtain

$$\Gamma^{(m)}(\boldsymbol{r}_1\sigma_1,\dots,\boldsymbol{r}_m\sigma_m;\boldsymbol{r}'_1\sigma'_1,\dots,\boldsymbol{r}'_m\sigma'_m) \equiv \frac{N!}{(N-m)!}\int \mathrm{d}x_{m+1}\dots\mathrm{d}x_N \times\Psi^*_{N;0}(\boldsymbol{r}_1\sigma_1,\dots,\boldsymbol{r}_m\sigma_m,x_{m+1},\dots,x_N) \times\Psi_{N;0}(\boldsymbol{r}'_1\sigma'_1,\dots,\boldsymbol{r}'_m\sigma'_m,x_{m+1},\dots,x_N), \quad \text{(B8)}$$

where we have permutated the coordinates of the wavefunctions and moreover introduced the following shorthand notation:

$$x_i{:=}\boldsymbol{r}_i\,\sigma_i, \qquad \int \mathrm{d}x_i\;(\dots){:=}\sum_{\sigma_i}\int \mathrm{d}^d r_i\;(\dots). \quad \text{(B9)}$$

In the two cases corresponding to $m = N-1$ and $m = N$, the integral on the RHS of Eq. (B8) should be understood as signifying the following: for the case $m = N-1$, $\int \mathrm{d}x_{m+1}\dots\mathrm{d}x_N \Rightarrow \int \mathrm{d}x_N$, and for the case $m = N$, $\int \mathrm{d}x_{m+1}\dots\mathrm{d}x_N \Rightarrow 1$ (i.e. *no* integration at all). From Eq. (B8) we can consistently define

$$\Gamma^{(0)} = 1 \quad (\Gamma^{(0)} \text{ has } \textit{no} \text{ arguments}). \quad \text{(B10)}$$

From Eq. (B8) we further deduce the following rule of contraction

$$\int \mathrm{d}x_m\;\Gamma^{(m)}(x_1,\dots,x_m;x'_1,\dots,x_m) = (N-m+1)\,\Gamma^{(m-1)}(x_1,\dots,x_{m-1};x'_1,\dots,x'_{m-1}), \quad m \ge 1. \quad \text{(B11)}$$

For fermion wavefunctions $\Psi_{N;0}(x_1,\dots,x_N)$, the odd-parity (even-parity) permutations of $\{x_1,\dots,x_N\}$ (do not) change the sign of $\Psi_{N;0}(x_1,\dots,x_N)$, from which, making use of the expression in Eq. (B8), the following relationships are immediately deduced:

$$\Gamma^{(m)}(x_1,\dots,x_j,\dots,x_i,\dots,x_m;x'_1,\dots,x'_m) = \mp\Gamma^{(m)}(x_1,\dots,x_i,\dots,x_j,\dots,x_m;x'_1,\dots,x'_m),$$
$$\Gamma^{(m)}(x_1,\dots,x_m;x'_1,\dots,x'_j,\dots,x'_i,\dots,x'_m) = \mp\Gamma^{(m)}(x_1,\dots,x_m;x'_1,\dots,x'_i,\dots,x'_j,\dots,x'_m), \quad \text{(B12)}$$

[119] From Eq. (158), one observes, however, that for systems composed of finite number of particles and localized in a finite region of space around the origin, such as atoms and molecules, $\hat{\psi}_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle$ up to normalization asymptotically approaches an $(N-1)$-particle *eigenstate* of $\widehat{H}$ for $\|\boldsymbol{r}\| \to \infty$; in contrast with what the pertinent equations might suggest at the first glance, the eigenvalue corresponding to this $(N-1)$-particle eigenstate *is* larger than $E_{N;0}$, following the fact that $E_{N-1;s} \ge E_{N-1;0}$ and that the first ionization potential $I_1{:=}E_{N-1;0}-E_{N;0}$ is positive (as an aside we note that the smallest I_1 for elements in the periodic table amounts to 3.89 eV, pertaining to the element Cs (Perdew, *et al.* 1982)).

depending on whether $x_i \rightleftharpoons x_j$ and $x'_i \rightleftharpoons x'_j$ correspond to odd-parity (upper signs) or even-parity (lower signs) permutations.

Since by assumption $\Psi_{N;0}(x_1,\dots,x_N)$ is real-valued (see above), from Eq. (B8) we observe that $\Gamma^{(m)}(\{x_i\};\{x'_i\})$, which in general is complex-valued and transforms into the conjugate value of the latter function upon the exchange $\{x_i\} \rightleftharpoons \{x'_i\}$, is in our considerations real-valued and thus satisfies

$$\Gamma^{(m)}(x'_1,\dots,x'_m;x_1,\dots,x_m) \equiv \Gamma^{(m)}(x_1,\dots,x_m;x'_1,\dots,x'_m). \tag{B13}$$

It can be easily verified that, for the *uniform* GSs of homogeneous systems, the following shift property holds:

$$\Gamma^{(m)}(\tilde{\boldsymbol{r}}_1\sigma_1,\dots,\tilde{\boldsymbol{r}}_m\sigma_m;\tilde{\boldsymbol{r}}'_1\sigma'_1,\dots,\tilde{\boldsymbol{r}}'_m\sigma'_m) \equiv \Gamma^{(m)}(\boldsymbol{r}_1\sigma_1,\dots,\boldsymbol{r}_m\sigma_m;\boldsymbol{r}'_1\sigma'_1,\dots,\boldsymbol{r}'_m\sigma'_m), \tag{B14}$$

where

$$\tilde{\boldsymbol{r}}_i {:=} \boldsymbol{r}_i + \boldsymbol{r}_0, \quad \tilde{\boldsymbol{r}}'_i {:=} \boldsymbol{r}'_i + \boldsymbol{r}_0, \ \ \forall\, i, \tag{B15}$$

in which $\boldsymbol{r}_0$ stands for an arbitrary constant vector.

For some $(m,\{x_i\},\{x'_i\})$, $\Gamma^{(m)}(\{x_i\};\{x'_i\})$ coincides with well-known static correlation functions. Three of these that feature in our present work are as follows.

(i) The partial density matrix

$$\varrho_\sigma(\boldsymbol{r},\boldsymbol{r}') {:=} \langle \Psi_{N;0}|\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}_\sigma(\boldsymbol{r}')|\Psi_{N;0}\rangle \equiv \Gamma^{(1)}(\boldsymbol{r}\sigma;\boldsymbol{r}'\sigma). \tag{B16}$$

(ii) Consequently, for the partial number density of particles with spin σ one has $n_\sigma(\boldsymbol{r}) \equiv \Gamma^{(1)}(\boldsymbol{r}\sigma;\boldsymbol{r}\sigma)$; note in passing that from Eq. (B2) we have $\Gamma^{(1)}(\boldsymbol{r}\sigma;\boldsymbol{r}'\sigma') \equiv 0$ for $\sigma \neq \sigma'$.

(iii) The van Hove (1954a,b) pair correlation function

$$\begin{aligned} g_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}') {:=} & \frac{1}{N(N-1)} \\ & \times \langle \Psi_{N;0}|\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}')\hat{\psi}_{\sigma'}(\boldsymbol{r}')\hat{\psi}_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle \\ \equiv & \frac{1}{N(N-1)}\,\Gamma^{(2)}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma'). \end{aligned} \tag{B17}$$

Following Eq. (B13), we have

$$\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \equiv \varrho_\sigma(\boldsymbol{r},\boldsymbol{r}') \tag{B18}$$

and, following Eq. (B12),

$$g_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}') \equiv g_{\sigma',\sigma}(\boldsymbol{r}',\boldsymbol{r}). \tag{B19}$$

For some applications it is meaningful to consider the following normalized van Hove pair correlation function:

$$\mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}') {:=} \Omega^2 g_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}'), \tag{B20}$$

which in the thermodynamic limit can be written as

$$\mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{n_0^2}\,\Gamma^{(2)}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma'), \tag{B21}$$

where n_0 stands for the *total* concentration of the particles, defined in Eq. (9).

For completeness we mention that the expression in Eq. (B8) can be deduced from that in Eq. (B1) through employing the following association between the second-quantized and first-quantized operators corresponding to N-particle systems;

$$\begin{aligned} \hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}_{\sigma'}(\boldsymbol{r}') \rightleftharpoons & \sum_{i=1}^{N} \delta_{\sigma,\sigma_i}\delta(\boldsymbol{r}-\boldsymbol{r}_i) \\ & \times \mathcal{P}^{\mathrm{op}}(\boldsymbol{r}',\boldsymbol{r}_i)\mathcal{S}^{\mathrm{op}}(\sigma',\sigma_i), \end{aligned} \tag{B22}$$

where the projection operators $\mathcal{P}^{\mathrm{op}}(\boldsymbol{r}',\boldsymbol{r}_i)$, $\mathcal{S}^{\mathrm{op}}(\sigma',\sigma_i)$ replace *all* $\boldsymbol{r}_i$ and σ_i to their rights by $\boldsymbol{r}'$ and σ' respectively. For illustration, we apply the prescription in Eq. (B22) to the van Hove pair correlation function as defined in Eq. (B17). To this end, from Eq. (B17), making use of the canonical anticommutation relations in Eq. (29), we first deduce that

$$\begin{aligned} N(N-1)g_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}') = & -\delta_{\sigma,\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}')\,n_\sigma(\boldsymbol{r}) \\ & + \langle \Psi_{N;0}|\hat{n}_\sigma(\boldsymbol{r})\hat{n}_{\sigma'}(\boldsymbol{r}')|\Psi_{N;0}\rangle, \end{aligned} \tag{B23}$$

where

$$\hat{n}_\sigma(\boldsymbol{r}) {:=} \hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}_\sigma(\boldsymbol{r}). \tag{B24}$$

From the prescription in Eq. (B22) it follows that

$$\begin{aligned} \langle \Psi_{N;0}|\hat{n}_\sigma(\boldsymbol{r})\hat{n}_{\sigma'}(\boldsymbol{r}')|\Psi_{N;0}\rangle = & \sum_{i=1}^{N}\sum_{j=1}^{N}\int \mathrm{d}x_1\dots\mathrm{d}x_N \\ & \times \Psi^*_{N;0}(x_1,\dots,x_N)\,\delta_{\sigma,\sigma_i}\,\delta(\boldsymbol{r}-\boldsymbol{r}_i) \\ & \times \delta_{\sigma',\sigma_j}\,\delta(\boldsymbol{r}'-\boldsymbol{r}_j)\,\Psi_{N;0}(x_1,\dots,x_N) \\ = \delta_{\sigma,\sigma'}\,\delta(\boldsymbol{r}-\boldsymbol{r}')\,n_\sigma(\boldsymbol{r}) + & N(N-1)\int \mathrm{d}x_3\dots\mathrm{d}x_N \\ & \times |\Psi_{N;0}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma',x_3,\dots,x_N)|^2, \end{aligned} \tag{B25}$$

which in combination with Eq. (B23) yields the expression for $g_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}')$ on the right-most side of Eq. (B17) in which $\Gamma^{(2)}$ is replaced by its configuration-space integral representation according to Eq. (B8). It should be noted that, in obtaining the RHS of Eq. (B25), we have first written

$$\sum_{i=1}^{N}\sum_{j=1}^{N} a_{ij} = \sum_{i=1}^{N} a_{ii} + \sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} a_{ij}, \tag{B26}$$

and subsequently made use of the invariance of $|\Psi_{N;0}(x_1,\dots,x_N)|$ under the permutation of its arguments; in this way, the sums have been replaced by the number of summands, namely

$$\sum_{i=1}^{N} 1 = N, \qquad \sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} 1 = N(N-1), \tag{B27}$$

times the value of a single summand.

Finally, for a concise notation, in the main text we employ the following auxiliary functions which all involve $\Gamma^{(2)}$:

$$\mathcal{A}(\boldsymbol{r},\boldsymbol{r}'){:=}\int \mathrm{d}^d r_1''\, \mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}'-\boldsymbol{r}_2'') \times \sum_{\sigma_1',\sigma_2'} \Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2';\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2'), \tag{B28}$$

$$\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}'){:=}\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'') \times \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}''\sigma',\boldsymbol{r}\sigma), \tag{B29}$$

$$\mathcal{C}(\boldsymbol{r},\boldsymbol{r}'){:=}\int \mathrm{d}^d r_1''\, \mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}'-\boldsymbol{r}_2'') \times \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}_1''\sigma',\boldsymbol{r}_2''\sigma';\boldsymbol{r}_1''\sigma',\boldsymbol{r}_2''\sigma'). \tag{B30}$$

One observes that $\mathcal{A}(\boldsymbol{r},\boldsymbol{r}')$ and $\mathcal{C}(\boldsymbol{r},\boldsymbol{r}')$ are directly related to the van Hove pair correlation function (see Eq. (B17) above), whereas this is the case for $\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ *only* when $\boldsymbol{r}=\boldsymbol{r}'$. We point out that calculations of $\mathcal{A}(\boldsymbol{r},\boldsymbol{r}')$, $\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and $\mathcal{C}(\boldsymbol{r},\boldsymbol{r}')$ corresponding to *extended* systems of fermions interacting through a long-range interaction function v have to be preceded by careful analyses of the long-distance asymptotic behaviours of the integrands on the RHSs of Eqs. (B28) - (B30). In Appendix F we carry out the necessary analyses for the specific case of $v \equiv v_c$ in $d=3$. In this context we identify the unbounded contributions to these functions and further establish the links between these and their counter-contributions that have their origins in other functions. For clarity of presentation, unless indicated or implied otherwise, in this work we denote the function obtained by removing the fundamentally unbounded part of an original function (defined in terms of an integral), by means of the symbol of the original function complemented by a single prime; thus, for instance, by $\mathcal{A}'(\boldsymbol{r},\boldsymbol{r}')$ we denote $\mathcal{A}(\boldsymbol{r},\boldsymbol{r}')$ bar its unbounded contribution (see Eqs. (F2) and (F73)). Without further specifying the details (which are sufficiently clearly indicated in the appropriate places in this paper), we draw attention to the fact that, in general, two and three primes attached to the symbol of an earlier-defined function similarly carry significance according to the notation adopted in this paper (see the Contents for a glimpse of such functions).

□

APPENDIX C: THE SINGLE SLATER-DETERMINANT APPROXIMATION (SSDA)

Approximating the interacting N-particle GS wavefunction $\Psi_{N;0}(x_1,\dots,x_N)$ by a SSD, which we denote by $\Phi_{N;0}(x_1,\dots,x_N)$, composed of N orthonormal one-particle spin-orbitals (in principle, these are the N normalized eigenfunctions $\varphi_{\varsigma;\sigma}(\boldsymbol{r})$ of Eq. (56) corresponding to the lowest N eigenvalues $\varepsilon_{\varsigma;\sigma}^{(0)}$; however, this aspect is of no fundamental significance to our considerations in this Appendix), results in considerable simplifications in the expressions derived and presented in this work. Viewed from the standpoint that gives especial prominence to interaction effects as manifested in the GS of interacting systems, a SSDA to $\Psi_{N;0}(x_1,\dots,x_N)$ is seen to be largely of interest through the fact that it provides *insight* into various aspects of often very complicated expressions. Interestingly however, some of the results deduced within the framework of the SSDA are *qualitatively* correct and in some instances are even amenable to being made *quantitatively* exact upon making a judicious choice for the 'non-interacting' many-body Hamiltonian $\widehat{H}_0$ of which $|\Phi_{N;0}\rangle$ is the N-particle GS. Below we first describe the procedure of calculating the m-particle correlation function $\Gamma^{(m)}(\{x_i\};\{x_i'\})$ within the framework of the SSDA, formally defined as follows (*cf.* Eq. (B1))

$$\Gamma_{\mathrm{s}}^{(m)}(\boldsymbol{r}_1\sigma_1,\dots,\boldsymbol{r}_m\sigma_m;\boldsymbol{r}_1'\sigma_1',\dots,\boldsymbol{r}_m'\sigma_m') {:=}\langle\Phi_{N;0}|\hat{\psi}_{\sigma_1}^{\dagger}(\boldsymbol{r}_1)\dots\hat{\psi}_{\sigma_m}^{\dagger}(\boldsymbol{r}_m) \times\hat{\psi}_{\sigma_m'}(\boldsymbol{r}_m')\dots\hat{\psi}_{\sigma_1'}(\boldsymbol{r}_1')|\Phi_{N;0}\rangle. \tag{C1}$$

Employing the expression for $\Gamma_{\mathrm{s}}^{(m)}(\{x_i\};\{x_i'\})$ in terms of the single-particle Slater-Fock density matrices $\{\Gamma_{\mathrm{s}}^{(1)}(x_i;x_j')\}$ (*cf.* Eq. (B16); see also Eq. (169)), we subsequently present the expressions within the framework of the SSDA of the correlation functions defined in the closing part of Appendix B. Before proceeding, we mention that in Appendix F (§ 1.c herein) we introduce the set of generalized density matrices $\Gamma_{\boldsymbol{\xi}}^{(m)}(\{x_i\};\{x_i'\})$ in terms of the complete set $\{|\boldsymbol{\xi}\rangle\}$ of N-particle Slater determinants; identifying $|\boldsymbol{\xi}=\boldsymbol{0}\rangle$ with $|\Phi_{N;0}\rangle$, we have

$$\Gamma_{\boldsymbol{\xi}=\boldsymbol{0}}^{(m)}(\{x_i\};\{x_i'\}) \equiv \Gamma_{\mathrm{s}}^{(m)}(\{x_i\};\{x_i'\}). \tag{C2}$$

In Appendix F we further encounter the so-called *transition* correlation function $\Gamma_{\boldsymbol{\xi},\boldsymbol{\xi}'}^{(m)}(\{x_i\};\{x_i'\})$ (McWeeny 1992, § 5.4) defined as follows:

$$\Gamma_{\boldsymbol{\xi},\boldsymbol{\xi}'}^{(m)}(\boldsymbol{r}_1\sigma_1,\dots,\boldsymbol{r}_m\sigma_m;\boldsymbol{r}_1'\sigma_1',\dots,\boldsymbol{r}_m'\sigma_m') {:=}\langle\boldsymbol{\xi}|\hat{\psi}_{\sigma_1}^{\dagger}(\boldsymbol{r}_1)\dots\hat{\psi}_{\sigma_m}^{\dagger}(\boldsymbol{r}_m) \times\hat{\psi}_{\sigma_m'}(\boldsymbol{r}_m')\dots\hat{\psi}_{\sigma_1'}(\boldsymbol{r}_1')|\boldsymbol{\xi}'\rangle. \tag{C3}$$

For the generalized m-point correlation function $\Gamma^{(m)}_{\boldsymbol{\xi}}$ we have

$$\Gamma^{(m)}_{\boldsymbol{\xi}}(\{x_i\};\{x_i'\}) := \Gamma^{(m)}_{\boldsymbol{\xi},\boldsymbol{\xi}}(\{x_i\};\{x_i'\}). \tag{C4}$$

The prescription that we present below for expressing $\Gamma_{\rm s}^{(m)}$ in terms of $\Gamma_{\rm s}^{(1)}$ (see Eq. (B16)), identically applies to $\Gamma^{(m)}_{\boldsymbol{\xi}}$, expressing this in terms of $\Gamma^{(1)}_{\boldsymbol{\xi}}$. For the general rules concerning determination of $\Gamma^{(m)}_{\boldsymbol{\xi},\boldsymbol{\xi}'}$, for $m = 1, 2$, in terms of simpler functions, we refer the reader to Eq. (5.4.14) of the book by McWeeny (1992). [120]

Within the framework of the SSDA, $\Gamma^{(m)}(\{x_i\};\{x_i'\})$ is fully expressed in terms of $\Gamma_{\rm s}^{(1)}(x;x') \equiv \delta_{\sigma,\sigma'}\ \Gamma_{\rm s}^{(1)}(\boldsymbol{r}\sigma;\boldsymbol{r}'\sigma) \equiv \delta_{\sigma,\sigma'}\ \varrho_{{\rm s};\sigma}(\boldsymbol{r},\boldsymbol{r}')$ (for example McWeeny 1992, pp. 125-128). This is easily demonstrated by employing the Laplace expansion of determinants, organized in such a way that the pertinent sub-determinants of order $(N-m)\times(N-m)$ do not involve functions with arguments $x_1,\dots,x_m$, $x_1',\dots,x_m'$; a subsequent use of the orthogonality of the corresponding $(N-m)$-particle Slater determinants, gives rise to the aforementioned simplification in the expression for $\Gamma_{\rm s}^{(m)}(\{x_i\};\{x_i'\})$; explicitly, in this expression, $\Gamma_{\rm s}^{(m)}(\{x_i\};\{x_i'\})$ is the determinant of an $m\times m$ matrix whose (i,j)th entry is equal to $\Gamma_{\rm s}^{(1)}(x_i;x_j') \equiv \delta_{\sigma_i,\sigma_j}\varrho_{{\rm s};\sigma_i}(\boldsymbol{r}_i,\boldsymbol{r}_j)$. [121] It is tempting to replace the latter Slater-Fock density matrix by its correlated counterpart $\varrho_{\sigma_i}(\boldsymbol{r}_i,\boldsymbol{r}_j)$ in order to regain, through the latter function, some of the lost correlation effects brought about by the SSDA. However, as $\varrho_{\sigma_i}(\boldsymbol{r}_i,\boldsymbol{r}_j)$, in contrast with $\varrho_{{\rm s};\sigma_i}(\boldsymbol{r}_i,\boldsymbol{r}_j)$, is *not* idempotent (i.e. whereas $\varrho_{{\rm s};\sigma}\varrho_{{\rm s};\sigma} \equiv \varrho_{{\rm s};\sigma}$, unless $v\equiv 0$, $\varrho_\sigma\varrho_\sigma \not\equiv \varrho_\sigma$), such a direct replacement gives rise to fundamentally erroneous results, such as incorrect values associated with the integrals of $\Gamma^{(m)}(\{x_i\};\{x_i'\})$ (see, for example, the text following Eq. (F11)).

Finally, we present the expressions for $\mathcal{A}(\boldsymbol{r},\boldsymbol{r}')$, $\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and $\mathcal{C}(\boldsymbol{r},\boldsymbol{r}')$, defined in Eqs. (B28), (B29) and (B30) respectively, within the SSDA scheme. Using the above prescription, we readily obtain

$$\mathcal{A}_{\rm s}(\boldsymbol{r},\boldsymbol{r}') = v_H(\boldsymbol{r};[n])v_H(\boldsymbol{r}';[n]) - \int {\rm d}^d r_1''\, {\rm d}^d r_2''\ v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}'-\boldsymbol{r}_2'')\sum_{\sigma'} \varrho^2_{{\rm s};\sigma'}(\boldsymbol{r}_1'',\boldsymbol{r}_2''), \tag{C5}$$

$$\mathcal{B}_{{\rm s};\sigma}(\boldsymbol{r},\boldsymbol{r}') = -v_H(\boldsymbol{r};[n])\varrho_{{\rm s};\sigma}(\boldsymbol{r}',\boldsymbol{r}) + \int {\rm d}^d r''\ v(\boldsymbol{r}-\boldsymbol{r}'')\varrho_{{\rm s};\sigma}(\boldsymbol{r}',\boldsymbol{r}'')\varrho_{{\rm s};\sigma}(\boldsymbol{r}'',\boldsymbol{r}), \tag{C6}$$

$$\mathcal{C}_{\rm s}(\boldsymbol{r},\boldsymbol{r}') = \sum_{\sigma'} v_H(\boldsymbol{r};[n_{\sigma'}])v_H(\boldsymbol{r}';[n_{\sigma'}]) - \int {\rm d}^d r_1''\, {\rm d}^d r_2''\ v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}'-\boldsymbol{r}_2'')\sum_{\sigma'} \varrho^2_{{\rm s};\sigma'}(\boldsymbol{r}_1'',\boldsymbol{r}_2''). \tag{C7}$$

On comparing the expressions in Eqs. (C5) and (C7), one readily deduces that

$$\mathcal{C}_{\rm s}(\boldsymbol{r},\boldsymbol{r}') \equiv \mathcal{A}_{\rm s}(\boldsymbol{r},\boldsymbol{r}') + \sum_{\sigma'} v_H(\boldsymbol{r};[n_{\sigma'}])v_H(\boldsymbol{r}';[n_{\sigma'}]) - v_H(\boldsymbol{r};[n])v_H(\boldsymbol{r}';[n]). \tag{C8}$$

Because of the close similarity between $\mathcal{A}(\boldsymbol{r},\boldsymbol{r}')$ and $\mathcal{C}(\boldsymbol{r},\boldsymbol{r}')$ (*cf.* Eqs. (B28) and (B30)), and specifically between their SSDA counterparts as exposed in Eq. (C8), the regularized expression for $\mathcal{C}(\boldsymbol{r},\boldsymbol{r}')$ appropriate to the case corresponding to $v\equiv v_c$ and $d=3$ is readily deduced along the lines of Appendix F. □

APPENDIX D: THE TIME-REVERSAL SYMMETRY AND THE VANISHING OF $\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}')$

In the most complete expression for $G_{\sigma;\infty_4}(\boldsymbol{r},\boldsymbol{r}')$ presented in Eq. (194), we encounter the GS correlation function

$$\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}') \equiv v(\boldsymbol{r}-\boldsymbol{r}')\,\gamma_\sigma(\boldsymbol{r},\boldsymbol{r}'), \tag{D1}$$

$$\gamma_\sigma(\boldsymbol{r},\boldsymbol{r}') := -\int {\rm d}^d r''\ v(\boldsymbol{r}'-\boldsymbol{r}'') \lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''} \tau(\boldsymbol{r}'') \times \sum_{\sigma'}\Big\{\Gamma^{(2)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}\sigma,\tilde{\boldsymbol{r}}''\sigma') - \Gamma^{(2)}(\boldsymbol{r}'\sigma,\tilde{\boldsymbol{r}}''\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma')\Big\}, \tag{D2}$$

which is seen to be asymmetric with respect to the exchange of $\boldsymbol{r}$ and $\boldsymbol{r}'$, in apparent contradiction with the required property $G_{\sigma;\infty_4}(\boldsymbol{r}',\boldsymbol{r}) \equiv G_{\sigma;\infty_4}(\boldsymbol{r},\boldsymbol{r}')$ (see Eq. (178)). Here we demonstrate that in fact

$$\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}') \equiv 0. \tag{D3}$$

As we shall see, the proof of this statement is more direct for systems with *non*-uniform GSs than for those with uniform GSs. In the course of obtaining the result in Eq. (D3), we encounter a direct relationship between $\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and a matrix element of the total paramagnetic flux-density operator $\hat{\boldsymbol{j}}_{\rm p}(\boldsymbol{r})$ with respect to an $(N_\sigma - 1 + N_{\bar\sigma})$-particle state directly associated with the $(N_\sigma + N_{\bar\sigma})$-particle GS of $\widehat{H}$. This relationship thus suggests a link between $\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}') \equiv 0$ and our assumption

[120] For completeness we indicate the following corrections to the mentioned Eq. (5.4.14): all functions $\psi_R'^*(\boldsymbol{x}_1)$ and $\psi_S'^*(\boldsymbol{x}_2)$ in this equation are to be replaced by $\psi^*_{R'}(\boldsymbol{x}_1)$ and $\psi^*_{S'}(\boldsymbol{x}_2)$ respectively (i.e. the primes pertain to the *subscripts* R and S and *not* to the spin-orbitals ψ_R and ψ_S); further, in (ii), $\pi(\kappa\lambda|\boldsymbol{x}_1,\boldsymbol{x}_1)$ is to be replaced by $\pi(\kappa\lambda|\boldsymbol{x}_1,\boldsymbol{x}_2)$.

[121] The validity of this prescription is readily verified by *incomplete induction*.

with regard to the non-degeneracy, and thus the time-reversal symmetry, of the GS of the system under consideration. [122]

From the defining expression for $\gamma_\sigma(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (D2), making use of the symmetry relation in Eq. (B13), it follows that

$$\gamma_\sigma(\boldsymbol{r},\boldsymbol{r}) \equiv 0, \tag{D4}$$

which we now show to have important implications for the integrand of the $\boldsymbol{r}''$ integral on the RHS of Eq. (D2). To this end, we first express $\gamma_\sigma(\boldsymbol{r},\boldsymbol{r}')$ as defined in Eq. (D2) in its most elementary form, namely

$$\gamma_\sigma(\boldsymbol{r},\boldsymbol{r}') \equiv \frac{\hbar^2}{2m_e}\langle\Psi_{N;0}|\hat{\psi}^\dagger_\sigma(\boldsymbol{r}') \times \sum_{\sigma'}\int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')\Big\{\big[\nabla^2_{\boldsymbol{r}''}\hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}'')\big]\hat{\psi}_{\sigma'}(\boldsymbol{r}'') - \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}'')\big[\nabla^2_{\boldsymbol{r}''}\hat{\psi}_{\sigma'}(\boldsymbol{r}'')\big]\Big\}\,\hat{\psi}_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle. \tag{D5}$$

Making use of

$$\big[\nabla^2 f(\boldsymbol{r})\big]g(\boldsymbol{r}) = \boldsymbol{\nabla}\cdot\big(\big[\boldsymbol{\nabla}f(\boldsymbol{r})\big]g(\boldsymbol{r})\big) - \big[\boldsymbol{\nabla}f(\boldsymbol{r})\big]\cdot\big[\boldsymbol{\nabla}g(\boldsymbol{r})\big] \tag{D6}$$

and the Gauss divergence theorem (or its equivalent in $d\neq 3$), we readily obtain

$$\gamma_\sigma(\boldsymbol{r},\boldsymbol{r}') \equiv i\hbar\int \mathrm{d}^d r''\;\big[\boldsymbol{\nabla}_{\boldsymbol{r}''} v(\boldsymbol{r}'-\boldsymbol{r}'')\big]\cdot \boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}'), \tag{D7}$$

where

$$\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}') := \langle\Psi_{N;0}|\hat{\psi}^\dagger_\sigma(\boldsymbol{r}')\,\hat{\boldsymbol{j}}_{\mathrm{p}}(\boldsymbol{r}'')\,\hat{\psi}_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle, \tag{D8}$$

with $\hat{\boldsymbol{j}}_{\mathrm{p}}(\boldsymbol{r}) \equiv \sum_\sigma \hat{\boldsymbol{j}}_{\mathrm{p};\sigma}(\boldsymbol{r})$ the *total* paramagnetic particle flux density operator, where

$$\hat{\boldsymbol{j}}_{\mathrm{p};\sigma}(\boldsymbol{r}) := \frac{-i\hbar}{2m_e}\Big\{\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\big[\boldsymbol{\nabla}_{\boldsymbol{r}}\hat{\psi}_\sigma(\boldsymbol{r})\big] - \big[\boldsymbol{\nabla}_{\boldsymbol{r}}\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\big]\hat{\psi}_\sigma(\boldsymbol{r})\Big\}. \tag{D9}$$

The expression in Eq. (D8) is the aforementioned direct relationship between $\mathcal{J}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ (see Eq. (D7)) and the matrix elements of the total paramagnetic flux density operator with respect to an $(N_\sigma-1+N_{\bar\sigma})$-particle state directly associated with the $(N_\sigma+N_{\bar\sigma})$-particle GS of $\widehat{H}$.

From Eq. (D8) it can be verified that

$$\Big(\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}')\Big)_\alpha \equiv \Big(\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r}',\boldsymbol{r})\Big)^*_\alpha,\;\; \alpha = x,y,\dots, \tag{D10}$$

that is $\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}')$ is Hermitian (here $\{\alpha\}$ denotes the components of *vector* $\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}')$ with respect to some d-dimensional basis). Since $\gamma_\sigma(\boldsymbol{r},\boldsymbol{r}')$ is real valued (see the defining expression in Eq. (D2) and consider our convention set out in the second paragraph of Appendix B), the property in Eq. (D10), which implies $\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r})$ to be real valued, in combination with Eq. (D7) leads to the conclusion that

$$\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}) \equiv 0,\;\; \forall \boldsymbol{r}'',\boldsymbol{r},\sigma;\quad \gamma_\sigma(\boldsymbol{r},\boldsymbol{r}) \equiv 0,\;\; \forall\boldsymbol{r},\sigma. \tag{D11}$$

The second of these results is exactly that directly obtained from the defining expression for $\gamma_\sigma(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (D2) and presented in Eq. (D4).

The Hermitian property of $\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}')$ implies that this function has the following spectral resolution: [123]

$$\Big(\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}')\Big)_\alpha = \sum_\varsigma \lambda^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}\, u^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}(\boldsymbol{r}) u^{(\alpha)*}_{\boldsymbol{r}''\sigma;\varsigma}(\boldsymbol{r}'), \tag{D12}$$

where $\lambda^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}$, a spectral point of $\Big(\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}')\Big)_\alpha$, is real and the spectral functions satisfy $\langle u^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}, u^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma'}\rangle = \delta_{\varsigma,\varsigma'}$; in principle the latter result applies when $\lambda^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma} \neq \lambda^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma'}$, however, in the case of degeneracy, the spectral functions can be made orthogonal through the Gram-Schmidt orthogonalization procedure. The representation in Eq. (D12) makes evident that for *non-uniform* states,

$$\Big(\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r})\Big)_\alpha \equiv 0,\; \forall\boldsymbol{r} \iff \lambda^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma} \equiv 0,\; \forall\varsigma. \tag{D13}$$

In other words, for *non-uniform* GSs, $\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}) \equiv \boldsymbol{0}$, $\forall\boldsymbol{r}$, suffices to establish that $\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}') \equiv \boldsymbol{0}$, $\forall\boldsymbol{r},\boldsymbol{r}'$. The essential role played by *non*-uniformity of the GS is that for these states the corresponding $\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}')$ is *not* a function of $\boldsymbol{r}-\boldsymbol{r}'$, so that $\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r})$ non-trivially depends on the *continuous* variable $\boldsymbol{r}$. Consequently, whereas it is possible that for *a given* $\boldsymbol{r}$ (or for a *finite* number of distinct $\boldsymbol{r}$) the set of $\lambda^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}$ can balance out the contributions of *all* $|u^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}(\boldsymbol{r})|^2$, resulting in a vanishing total contribution $\big(\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r})\big)_\alpha$ (see Eq. (D12)), the $\boldsymbol{r}$ *independence* of $\big\{\lambda^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}\big\}$, on the one hand, and the non-trivial dependence of $\big\{|u^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}(\boldsymbol{r})|^2\big\}$, on $\boldsymbol{r}$ on the other

[122] In the absence of an external magnetic field, the time-reversal symmetry can be broken only spontaneously; such type of broken-symmetry state can arise only in a manifold of degenerate GSs.

[123] We point out that, whereas the spectral content of $\big(\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}')\big)_\alpha$ is not exhausted solely by a point spectrum (i.e. by a set of 'eigenvalues'; see footnote 39), the spectral functions $\{u_{\boldsymbol{r}''\sigma;\varsigma}(\boldsymbol{r})\}$ are orthonormal and thus complete, as opposed to 'over-complete'.

hand (see further), do not allow for any other possibility but that presented in Eq. (D13). For clarity, it is here essential to realize that, even though $\boldsymbol{r}''$ is also a continuous variable, the dependence on $\boldsymbol{r}''$ of both $\{\lambda^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}\}$ and $\{|u^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}(\boldsymbol{r})|^2\}$ implies that the result in Eq. (D13) is *not* necessarily true for uniform systems where $\{|u^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}(\boldsymbol{r})|^2\}$ is *not* capable of being varied (through variation of the continuous variable $\boldsymbol{r}''$) independently from $\{\lambda^{(\alpha)}_{\boldsymbol{r}''\sigma;\varsigma}\}$.

Now we demonstrate that the result in Eq. (D13) holds true also for systems with uniform and isotropic GSs (the assumption concerning the isotropy of the GS is *not* essential to our arguments that follow; its relaxation, however, necessitates introduction of some additional symbols which we hereby avoid for simplicity but without loss of generality). To this end, we first point out that, for such systems, $\gamma_\sigma(\boldsymbol{r},\boldsymbol{r}') \equiv \gamma^{\rm h}_\sigma(\|\boldsymbol{r}-\boldsymbol{r}'\|)$ and $\boldsymbol{A}_{\boldsymbol{r}''\sigma}(\boldsymbol{r},\boldsymbol{r}') \equiv \boldsymbol{A}^{\rm h}_{\boldsymbol{r}''\sigma}(\|\boldsymbol{r}-\boldsymbol{r}'\|)$ (see Eq. (F9)), where on account of the result in Eq. (D11) we have $\gamma^{\rm h}_\sigma(0) = 0$ and $\boldsymbol{A}^{\rm h}_{\boldsymbol{r}''\sigma}(0) \equiv 0$. Thus for uniform systems, following a shift transformation in the variable of integration and application of the result $\boldsymbol{\nabla}_{\boldsymbol{r}''} v(\boldsymbol{r}-\boldsymbol{r}'') \equiv -\boldsymbol{\nabla}_{\boldsymbol{r}} v(\boldsymbol{r}-\boldsymbol{r}'')$, Eq. (D7) can be written as

$$\gamma^{\rm h}_\sigma(\|\delta\boldsymbol{r}\|) = \frac{\hbar}{i}\boldsymbol{\nabla}_{\boldsymbol{r}}\cdot\int {\rm d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\boldsymbol{A}^{\rm h}_{\boldsymbol{r}''+\delta\boldsymbol{r}\sigma}(\|\delta\boldsymbol{r}\|),\quad \forall\boldsymbol{r},\qquad \text{(D14)}$$

where $\delta\boldsymbol{r} := \boldsymbol{r}'-\boldsymbol{r}$ is an independent variable. The significance of this result lies in the fact that its LHS is independent of $\boldsymbol{r}$ whereas its RHS explicitly depends on $\boldsymbol{r}$. For cases where $v(\boldsymbol{r}-\boldsymbol{r}'')$ is short range, it is evident from Eq. (D14) that, for sufficiently large $\|\boldsymbol{r}\|$, to leading order in $1/\|\boldsymbol{r}\|$ the integral on the RHS of Eq. (D14) is proportional to $\boldsymbol{\nabla}_{\boldsymbol{r}}\cdot\boldsymbol{A}^{\rm h}_{\boldsymbol{r}+\delta\boldsymbol{r}\sigma}(\|\delta\boldsymbol{r}\|)$, which in combination with the independence of the LHS results in the conclusion that

$$\gamma^{\rm h}_\sigma(r) \equiv 0,\quad \forall r. \qquad \text{(D15)}$$

For the long-range Coulomb interaction in $d=3$, using the multi-pole expansion of this function (see Eq. (F20)), one observes that the RHS of Eq. (D14) is a power-low decaying function for $\|\boldsymbol{r}\|\to\infty$, which by the same reasoning as above, results in the conclusion presented in Eq. (D15). We thus arrive at the conclusion that the expression in Eq. (D13) applies to all systems, irrespective of whether the corresponding GSs are uniform or otherwise. □

APPENDIX E: SYMMETRY OF SOME CORRELATION FUNCTIONS

In the main text we encounter some two-point correlation functions, here denoted by, for example, $f(\boldsymbol{r},\boldsymbol{r}')$, which belong to one of the following categories:

(i) explicitly symmetric, that is those functions that *directly* transform into themselves upon effecting the exchange $\boldsymbol{r}\rightleftharpoons\boldsymbol{r}'$;

(ii) asymmetric functions (such as $f(\boldsymbol{r},\boldsymbol{r}')$) that occur in pairs, $f(\boldsymbol{r},\boldsymbol{r}')+f(\boldsymbol{r}',\boldsymbol{r})$, one transforming into another upon applying $\boldsymbol{r}\rightleftharpoons\boldsymbol{r}'$;

(iii) explicitly asymmetric functions that, however, can be shown to be symmetric upon some algebraic manipulation;

(iv) functions (such as $f_1(\boldsymbol{r},\boldsymbol{r}')$) that are nonsymmetric but that can be shown to lead to symmetric functions in combination with other equally nonsymmetric functions (such as $f_2(\boldsymbol{r},\boldsymbol{r}')$, with $f_1(\boldsymbol{r},\boldsymbol{r}')+f_2(\boldsymbol{r},\boldsymbol{r}')$ symmetric);

(v) functions that are explicitly asymmetric but detailed considerations reveal these to be identically vanishing.

In Appendix D we deal with the only function of the latter category that one encounters in considerations of $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ with m limited to $0,1$ and 2. In this Appendix we consider functions from categories (iii) and (iv).

1. Implicitly symmetric functions

Consider

$$\mathcal{I}_\sigma(\boldsymbol{r},\boldsymbol{r}') := \int {\rm d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'') \lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''} \tau(\boldsymbol{r}'') \times v(\boldsymbol{r}-\boldsymbol{r}'')\sum_{\sigma'}\Gamma^{(2)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}\sigma,\tilde{\boldsymbol{r}}''\sigma'). \qquad \text{(E1)}$$

Using the definition for $\Gamma^{(2)}$ in Eq. (B1), the expression in Eq. (E1) is readily brought into the following elementary form

$$\mathcal{I}_\sigma(\boldsymbol{r},\boldsymbol{r}') = -\langle\Psi_{N;0}|\hat{\psi}^\dagger_\sigma(\boldsymbol{r}')\sum_{\sigma'}\int {\rm d}^d r''\,\Big\{v(\boldsymbol{r}'-\boldsymbol{r}'') \times\big[\tau(\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'')\hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}'')\big]\hat{\psi}_{\sigma'}(\boldsymbol{r}'')\Big\}\hat{\psi}_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle. \qquad \text{(E2)}$$

Through applying the Gauss divergence theorem (or its equivalent in $d\neq 3$), one readily obtains

$$\mathcal{I}_\sigma(\boldsymbol{r},\boldsymbol{r}') = -\langle\Psi_{N;0}|\hat{\psi}^\dagger_\sigma(\boldsymbol{r}')\sum_{\sigma'}\int {\rm d}^d r''\,\Big\{v(\boldsymbol{r}-\boldsymbol{r}'') \times\hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}'')\big[\tau(\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\hat{\psi}_{\sigma'}(\boldsymbol{r}'')\big]\Big\}\hat{\psi}_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle \equiv \mathcal{I}^*_\sigma(\boldsymbol{r}',\boldsymbol{r}). \qquad \text{(E3)}$$

Since $\mathcal{I}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ is real-valued (see the second paragraph in Appendix B), the result in Eq. (E3) demonstrates the symmetry of $\mathcal{I}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ with respect to $\boldsymbol{r}\rightleftharpoons\boldsymbol{r}'$.

In a similar fashion as above, one can also deduce that (here $\mathcal{I}_\sigma$ is merely a generic symbol for functions defined in terms of integrals)

$$\mathcal{I}_\sigma(\boldsymbol{r},\boldsymbol{r}'):=\int \mathrm{d}^d r''\; v(\boldsymbol{r}'-\boldsymbol{r}'')\lim_{\tilde{\boldsymbol{r}}''\to\boldsymbol{r}''}\tau(\boldsymbol{r}'') \times v(\boldsymbol{r}-\boldsymbol{r}'')\sum_{\sigma'}\Gamma^{(2)}(\boldsymbol{r}'\sigma,\tilde{\boldsymbol{r}}''\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma') \qquad \text{(E4)}$$

is symmetric, that is $\mathcal{I}_\sigma(\boldsymbol{r}',\boldsymbol{r})\equiv\mathcal{I}_\sigma(\boldsymbol{r},\boldsymbol{r}')$. □

2. Asymmetric functions $\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')$, $\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and their symmetric combinations $\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and $\mathcal{F}_\sigma(\boldsymbol{r},\boldsymbol{r}')$

The function $\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ as defined in Eq. (B29) is evidently asymmetric. Here we demonstrate that

$$\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}'):=h_0(\boldsymbol{r})\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})-\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}') \qquad \text{(E5)}$$

is symmetric. To this end we consider the equation of motion for the annihilation field operator $\hat{\psi}_\sigma(\boldsymbol{r}t)$ in the Heisenberg picture (Fetter and Walecka 1971, p. 59) (see footnote 44)

$$\big[i\hbar\frac{\mathrm{d}}{\mathrm{d}t}-h_0(\boldsymbol{r})\big]\hat{\psi}_\sigma(\boldsymbol{r}t)=\sum_{\sigma'}\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'') \times\hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}''t)\hat{\psi}_{\sigma'}(\boldsymbol{r}''t)\hat{\psi}_\sigma(\boldsymbol{r}t), \qquad \text{(E6)}$$

where we have employed the Hamiltonian $\widehat{H}$ in Eqs. (1) and (2)and the equal-time anticommutation relations for the Heisenberg-picture field operators, which are identical with those in Eq. (29) which concern the Schrödinger-picture field-operators. Multiplying both sides of Eq. (E6) from the left by $\hat{\psi}^\dagger_\sigma(\boldsymbol{r}'t')$, with $t'>t$, taking the expectation value of the resulting equation with respect to $|\Psi_{N;0}\rangle$, from the definition of the single-particle GF $G_\sigma(\boldsymbol{r}t,\boldsymbol{r}'t')$, namely

$$G_\sigma(\boldsymbol{r}t,\boldsymbol{r}'t'):=-i\,\langle\Psi_{N;0}|\mathrm{T}\big\{\hat{\psi}_\sigma(\boldsymbol{r}t)\hat{\psi}^\dagger_\sigma(\boldsymbol{r}'t')\big\}|\Psi_{N;0}\rangle, \qquad \text{(E7)}$$

where T stands for the fermion time-ordering operator (Fetter and Walecka 1971, p. 65), we obtain

$$-i\big[i\hbar\frac{\mathrm{d}}{\mathrm{d}t}-h_0(\boldsymbol{r})\big]G_\sigma(\boldsymbol{r}t,\boldsymbol{r}'t')=\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'') \times\sum_{\sigma'}\langle\Psi_{N;0}|\hat{\psi}^\dagger_\sigma(\boldsymbol{r}'t')\hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}''t)\hat{\psi}_{\sigma'}(\boldsymbol{r}''t)\hat{\psi}_\sigma(\boldsymbol{r}t)|\Psi_{N;0}\rangle, \quad t'>t. \qquad \text{(E8)}$$

Now we employ the Fourier representation

$$G_\sigma(\boldsymbol{r}t,\boldsymbol{r}'t')=\int_{-\infty}^{\infty}\frac{\mathrm{d}\varepsilon}{2\pi\hbar}\,\mathrm{e}^{-i\varepsilon(t-t')/\hbar}\,G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon), \qquad \text{(E9)}$$

from which we obtain (below $\eta\downarrow 0$, corresponds to $t'\downarrow t$)

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\,G_\sigma(\boldsymbol{r}t,\boldsymbol{r}'t')|_{t'\downarrow t}=\frac{i}{\hbar}\int_{-\infty}^{\infty}\frac{\mathrm{d}\varepsilon}{2\pi i}\,\mathrm{e}^{i\varepsilon\eta/\hbar}\,\varepsilon\,G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon), \qquad \text{(E10)}$$

$$-i\,G_\sigma(\boldsymbol{r}t,\boldsymbol{r}'t')|_{t'\downarrow t}=\frac{1}{\hbar}\int_{-\infty}^{\infty}\frac{\mathrm{d}\varepsilon}{2\pi i}\,\mathrm{e}^{i\varepsilon\eta/\hbar}\,G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon) \equiv\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}). \qquad \text{(E11)}$$

Upon taking the limit $t'\downarrow t$ on both sides of Eq. (E8) and making use of the results in Eqs. (E10) and (E11), we obtain (see Eq. (B29))

$$\frac{1}{\hbar}\int_{-\infty}^{\infty}\frac{\mathrm{d}\varepsilon}{2\pi i}\,\mathrm{e}^{i\varepsilon\eta/\hbar}\big[\varepsilon-h_0(\boldsymbol{r})\big]G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon) =\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\sum_{\sigma'}\Gamma^{(2)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma') \equiv-\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}'), \qquad \text{(E12)}$$

from which, making use of Eq. (E11), we deduce (*cf.* Eq. (E5))

$$h_0(\boldsymbol{r})\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})-\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}')\equiv\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}') =\frac{1}{\hbar}\int_{-\infty}^{\infty}\frac{\mathrm{d}\varepsilon}{2\pi i}\,\mathrm{e}^{i\varepsilon\eta/\hbar}\,\varepsilon\,G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon). \qquad \text{(E13)}$$

Since $G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)\equiv G_\sigma(\boldsymbol{r}',\boldsymbol{r};\varepsilon)$ (for a detailed demonstration see Farid (1999a)), Eq. (E13) establishes that indeed

$$\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}')\equiv\mathcal{D}_\sigma(\boldsymbol{r}',\boldsymbol{r}). \qquad \text{(E14)}$$

For completeness, we mention that, through employing the Lehmann representation in Eq. (17) and application of the residue theorem, from the right-most expression on the RHS of Eq. (E13) one obtains

$$\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}')\equiv\sum_s^{<}\varepsilon_{s;\sigma}f_{s;\sigma}(\boldsymbol{r})f^*_{s;\sigma}(\boldsymbol{r}'), \qquad \text{(E15)}$$

where $\sum_s^<$ denotes the sum over *all* s for which $\varepsilon_{s;\sigma}<\mu$ holds (see Eq. (168) and the succeeding text). We note in passing that, from Eq. (E5), making use of Eq. (43), one readily obtains

$$u(\boldsymbol{r})=\frac{1}{n(\boldsymbol{r})}\sum_\sigma\Big\{\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r})+\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}) -\lim_{\boldsymbol{r}'\to\boldsymbol{r}}\tau(\boldsymbol{r})\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\Big\}. \qquad \text{(E16)}$$

This expression is of conceptual relevance in exposing the one-to-one correspondence between $u(\boldsymbol{r})$ and $n(\boldsymbol{r})$ corresponding to non-degenerate GSs of many-particle systems, as expected through a theorem due to Hohenberg and Kohn (1964). [124] It is important to realize

[124] According to this theorem, $u(\boldsymbol{r})$ is *up to a constant* uniquely determined by $n(\boldsymbol{r})$; this aspect is not reflected in the

that, for the expression in Eq. (E16) not to reduce into an *identity*, it is important that $\mathcal{B}_\sigma$ herein be calculated from the defining expression in Eq. (B29) and $\mathcal{D}_\sigma$ from the right-most expression on the RHS of Eq. (E13). The result in Eq. (E16) may be employed for the purpose of verifying the correctness and establishing the accuracy of the (numerically) calculated functions n, ϱ_σ, $\mathcal{B}_\sigma$ and $\mathcal{D}_\sigma$ in applications of the formalism described in this paper.

It is sometimes advantageous to make the symmetry property in Eq. (E14) explicit by means of symmetrizing the RHS of Eq. (E5), thus obtaining

$$\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{2}\big[h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}')\big]\, \varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) - \frac{1}{2}\big[\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}') + \mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big]. \tag{E17}$$

A second non-symmetric function of $\boldsymbol{r}$ and $\boldsymbol{r}'$ encountered in the main text is the following

$$\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}') := \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'') \times \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma') + \int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_2'') \times \sum_{\sigma_1',\sigma_2'} \Gamma^{(3)}(\boldsymbol{r}'\sigma,\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2';\boldsymbol{r}\sigma,\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2'). \tag{E18}$$

We now determine the counter-terms which in combination with this function give rise to a *symmetric* function. To this end we proceed from the Heisenberg equation of motion in Eq. (E6) above. Multiplying both sides of this equation from left by $[i\hbar\mathrm{d}/\mathrm{d}t - h_0(\boldsymbol{r})]\hat{\psi}_\sigma^\dagger(\boldsymbol{r}'t')$, replacing $[i\hbar\mathrm{d}/\mathrm{d}t - h_0(\boldsymbol{r})]\hat{\psi}_\sigma(\boldsymbol{r}t)$ on the RHS of the thus-obtained equation by the RHS of Eq. (E6) followed by a normal-ordering of the equal-time Heisenberg field operators, we obtain

$$\big[i\hbar\frac{\mathrm{d}}{\mathrm{d}t} - h_0(\boldsymbol{r})\big]^2 \hat{\psi}_\sigma^\dagger(\boldsymbol{r}'t')\hat{\psi}_\sigma(\boldsymbol{r}t) = \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}-\boldsymbol{r}'') \times \sum_{\sigma'} \hat{\psi}_\sigma^\dagger(\boldsymbol{r}'t')\hat{\psi}_{\sigma'}^\dagger(\boldsymbol{r}''t)\hat{\psi}_{\sigma'}(\boldsymbol{r}''t)\hat{\psi}_\sigma(\boldsymbol{r}t) + \int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_2'') \times \sum_{\sigma_1',\sigma_2'} \hat{\psi}_\sigma^\dagger(\boldsymbol{r}'t')\hat{\psi}_{\sigma_1'}^\dagger(\boldsymbol{r}_1''t)\hat{\psi}_{\sigma_2'}^\dagger(\boldsymbol{r}_2''t) \times \hat{\psi}_{\sigma_2'}(\boldsymbol{r}_2''t)\hat{\psi}_\sigma(\boldsymbol{r}_1''t)\hat{\psi}_\sigma(\boldsymbol{r}t). \tag{E19}$$

Along similar lines as above, that is by taking the expectation value of both sides of Eq. (E19) with respect to $|\Psi_{N;0}\rangle$ and subsequently taking the limit $t' \downarrow t$, we arrive at

$$\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}') = \mathcal{F}_\sigma(\boldsymbol{r},\boldsymbol{r}') - 2h_0(\boldsymbol{r})\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}') + h_0(\boldsymbol{r})h_0(\boldsymbol{r})\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}), \tag{E20}$$

where (below $\eta \downarrow 0$)

$$\mathcal{F}_\sigma(\boldsymbol{r},\boldsymbol{r}') := \frac{1}{\hbar}\int_{-\infty}^{\infty} \frac{\mathrm{d}\varepsilon}{2\pi i}\, \mathrm{e}^{i\varepsilon\eta/\hbar}\, \varepsilon^2\, G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon) \equiv -i\left(i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 G_\sigma(\boldsymbol{r}t,\boldsymbol{r}'t')\big|_{t'\downarrow t}. \tag{E21}$$

Here again $G_\sigma(\boldsymbol{r}',\boldsymbol{r};\varepsilon) \equiv G_\sigma(\boldsymbol{r},\boldsymbol{r}';\varepsilon)$ (Farid 1999a) implies that $\mathcal{F}_\sigma(\boldsymbol{r}',\boldsymbol{r}) \equiv \mathcal{F}_\sigma(\boldsymbol{r},\boldsymbol{r}')$. From Eq. (E20) we have the combination of functions that together with the asymmetric function $\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ result in a symmetric function, namely $\mathcal{F}_\sigma(\boldsymbol{r},\boldsymbol{r}')$. Similar to the expression for $\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (E17), the following symmetrized expression brings out the true symmetry of $\mathcal{F}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and may be employed in applications

$$\begin{aligned}\mathcal{F}_\sigma(\boldsymbol{r},\boldsymbol{r}') &= \frac{1}{2}\big[\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}') + \mathcal{G}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big] + \big[h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}')\big]\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r}') - \frac{1}{2}\big[h_0(\boldsymbol{r})h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}')h_0(\boldsymbol{r}')\big]\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \\ &\equiv \frac{1}{2}\big[\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}') + \mathcal{G}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big] + h_0(\boldsymbol{r})h_0(\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) - \frac{1}{2}\big[h_0(\boldsymbol{r}) + h_0(\boldsymbol{r}')\big]\,\big[\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}') + \mathcal{B}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big].\end{aligned} \tag{E22}$$

□

APPENDIX F: REGULARIZATION OF SOME CORRELATION FUNCTIONS PERTAINING TO COULOMB-INTERACTING FERMION SYSTEMS

Some essential integrals in our present work involving the correlation functions $\Gamma^{(m)}(\{x_i\};\{x_i'\})$, $m = 2, 3$, and the long-range Coulomb potential v_c in $d = 3$, are *not* well-defined in the thermodynamic limit. In this Appendix we deduce and present the regularized forms of these integrals which can be directly employed and numerically evaluated.

1. $\mathcal{A}(\boldsymbol{r},\boldsymbol{r}')$ and its regularized form; $\mathcal{A}'(\boldsymbol{r},\boldsymbol{r}')$

a. Arbitrary systems

Consider $\mathcal{A}(\boldsymbol{r},\boldsymbol{r}')$ as defined in Eq. (B28). Making use of the anticommutation relations in Eq. (29), we readily obtain

---

expression in Eq. (E16) (i.e. there is *no* arbitrariness in this expression) because in our considerations we have assumed the GS wavefunction to be real-valued, whereby we have fixed the global gauge in the problem under consideration (see the second paragraph in Appendix B).

$$
\begin{aligned}
&\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'; \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2') \\
&\quad = -\delta_{\sigma_1',\sigma_2'}\, \delta(\boldsymbol{r}_1'' - \boldsymbol{r}_2'')\, n_{\sigma_1'}(\boldsymbol{r}_1'') + n_{\sigma_1'}(\boldsymbol{r}_1'') n_{\sigma_2'}(\boldsymbol{r}_2'') \\
&\quad\quad + \langle \Psi_{N;0} | \big[\hat{n}_{\sigma_1'}(\boldsymbol{r}_1'') - n_{\sigma_1'}(\boldsymbol{r}_1'')\big] \\
&\quad\quad\quad \times \big[\hat{n}_{\sigma_2'}(\boldsymbol{r}_2'') - n_{\sigma_2'}(\boldsymbol{r}_2'')\big] | \Psi_{N;0} \rangle. \qquad \text{(F1)}
\end{aligned}
$$

Substitution of this expression in the RHS of Eq. (B28) yields (see text following Eq. (15) in § II.A concerning our convention with regard to v and v')

$$
\begin{aligned}
&\mathcal{A}(\boldsymbol{r}, \boldsymbol{r}') = v_H(\boldsymbol{r}; [n])\, v_H(\boldsymbol{r}'; [n]) \\
&\quad - \int \mathrm{d}^d r''\; v(\boldsymbol{r} - \boldsymbol{r}'') v(\boldsymbol{r}' - \boldsymbol{r}'')\, n(\boldsymbol{r}'') + \mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}'), \quad \text{(F2)}
\end{aligned}
$$

where

$$
\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}') := \int \mathrm{d}^d r_1'' \mathrm{d}^d r_2''\; v(\boldsymbol{r} - \boldsymbol{r}_1'') v(\boldsymbol{r}' - \boldsymbol{r}_2'') \mathcal{U}(\boldsymbol{r}_1'', \boldsymbol{r}_2''), \quad \text{(F3)}
$$

in which

$$
\begin{aligned}
\mathcal{U}(\boldsymbol{r}_1'', \boldsymbol{r}_2'') := \sum_{\sigma_1', \sigma_2'} &\langle \Psi_{N;0} | \big[\hat{n}_{\sigma_1'}(\boldsymbol{r}_1'') - n_{\sigma_1'}(\boldsymbol{r}_1'')\big] \\
&\times \big[\hat{n}_{\sigma_2'}(\boldsymbol{r}_2'') - n_{\sigma_2'}(\boldsymbol{r}_2'')\big] | \Psi_{N;0} \rangle. \quad \text{(F4)}
\end{aligned}
$$

In $d = 3$ and for $v \equiv v_c$, the Coulomb potential, neither

$$
v_H(\boldsymbol{r}; [n_0])\, v_H(\boldsymbol{r}'; [n_0])
$$

nor

$$
-n_0 \int \mathrm{d}^3 r''\; v(\boldsymbol{r} - \boldsymbol{r}'') v(\boldsymbol{r}' - \boldsymbol{r}'')
$$

exists for $\kappa \downarrow 0$; here n_0 stands for the total concentration of fermions defined in Eq. (9). Further, as the former contribution depends *quadratically* upon n_0 while the latter *linearly* upon n_0, it is evident that these contributions cannot cancel so that for the case under consideration, either $\mathcal{A}(\boldsymbol{r}, \boldsymbol{r}')$ is unbounded or otherwise $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ must contain contributions that remove the indicated unbounded contributions. Before presenting details, demonstrating that $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ *is* well-defined (i.e., it is *not* unbounded), we point out that the local part of $\Sigma_{\sigma;\infty_1}(\boldsymbol{r}, \boldsymbol{r}')$, that is $\Sigma^{\mathrm{l}}_{\sigma;\infty_1}(\boldsymbol{r}, \boldsymbol{r}')$ as presented in Eq. (187), is *exactly* equal to $\hbar^{-1} \mathcal{A}'(\boldsymbol{r}, \boldsymbol{r})\, \delta(\boldsymbol{r} - \boldsymbol{r}')$ so that the possible unboundedness of $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r})$ would amount to the result that in the AS of $\widetilde{\Sigma}_\sigma(\boldsymbol{r}, \boldsymbol{r}'; z)$ for $|z| \to \infty$, the leading asymptotic term following the constant $\Sigma_{\sigma;\infty_0}(\boldsymbol{r}, \boldsymbol{r}')$, would not be of the form $\Sigma_{\sigma;\infty_1}(\boldsymbol{r}, \boldsymbol{r}')/z$, but that this would be preceded by a more dominant term (see § II.B). In what follows we shall in the main focus on the case corresponding to $d = 3$ and $v \equiv v_c$.

We now demonstrate that $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ is *bounded* (in contrast, for $v \equiv v_c$ in $d = 2$, $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ turns out to be unbounded; B. Farid, 2001, unpublished). To this end, we first point out that

$$
\int \mathrm{d}^d r_1''\; \mathcal{U}(\boldsymbol{r}_1'', \boldsymbol{r}_2'') \equiv \int \mathrm{d}^d r_2''\; \mathcal{U}(\boldsymbol{r}_1'', \boldsymbol{r}_2'') \equiv 0, \qquad \text{(F5)}
$$

which follow from the combination of the following facts.

(i) $\sum_{\sigma'} \int \mathrm{d}^d r'\; \hat{n}_{\sigma'}(\boldsymbol{r}') = \widehat{N}$, the *total* number operator.

(ii) $|\Psi_{N;0}\rangle$ is an eigenstate of $\widehat{N}$.

(iii) $\sum_{\sigma'} \int \mathrm{d}^d r'\; n_{\sigma'}(\boldsymbol{r}') = N$.

For large values of $\|\boldsymbol{r}\|$ and $\|\boldsymbol{r}'\|$, employing the asymptotic results $v_c(\boldsymbol{r} - \boldsymbol{r}'') \sim v_c(\boldsymbol{r}) \propto 1/\|\boldsymbol{r}\|$ and $v_c(\boldsymbol{r}' - \boldsymbol{r}'') \sim v_c(\boldsymbol{r}') \propto 1/\|\boldsymbol{r}'\|$ in the integrand on the RHS of Eq. (F3), we arrive at the conclusion that $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}') \sim 0$ to orders $1/\|\boldsymbol{r}\|$ and $1/\|\boldsymbol{r}'\|$, as $\|\boldsymbol{r}\|, \|\boldsymbol{r}'\| \to \infty$. This result in particular implies that $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ *cannot* involve a *constant* unbounded contribution under the conditions considered in this Appendix. In contrast, $v_H(\boldsymbol{r}; [n_0])$ and $v_H(\boldsymbol{r}'; [n_0])$ diverge for *all* $\boldsymbol{r}$ and $\boldsymbol{r}'$ as $\kappa \downarrow 0$ (see Eq. (15)). We point out that for uniform and isotropic systems, $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ is a function of $\|\boldsymbol{r} - \boldsymbol{r}'\|$, so that in these systems $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}') \sim 0$ to order $1/\|\boldsymbol{r} - \boldsymbol{r}'\|$ for $\|\boldsymbol{r} - \boldsymbol{r}'\| \to \infty$. It is important to take this fact into account when considering uniform GSs, since in these the conditions $\|\boldsymbol{r}\|, \|\boldsymbol{r}'\| \to \infty$ do *not* necessarily imply $\|\boldsymbol{r} - \boldsymbol{r}'\| \to \infty$.

Now, making use of Eq. (16), the application of $\nabla^2_{\boldsymbol{r}}$ and $\nabla^2_{\boldsymbol{r}'}$ from the left to $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ in Eq. (F3) yields

$$
\begin{aligned}
\nabla^2_{\boldsymbol{r}} \nabla^2_{\boldsymbol{r}'} \mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}') &= \big(-e^2/\epsilon_0\big)^2 \mathcal{U}(\boldsymbol{r}, \boldsymbol{r}') \\
&\equiv \big(-e^2/\epsilon_0\big)^2 \Big(\sum_{\sigma, \sigma'} \Gamma^{(2)}(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma'; \boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') \\
&\quad - n(\boldsymbol{r}) n(\boldsymbol{r}') + n(\boldsymbol{r})\, \delta(\boldsymbol{r} - \boldsymbol{r}') \Big), \quad \text{(F6)}
\end{aligned}
$$

where we have made use of Eqs. (F1) and (F4). From the definition of $\Gamma^{(2)}$ in Eq. (B1) it is evident that the first contribution enclosed by large parentheses on the RHS of Eq. (F6), similar to the second contribution, is bounded for *all* [125] $\boldsymbol{r}$ and $\boldsymbol{r}'$ so that $\nabla^2_{\boldsymbol{r}} \nabla^2_{\boldsymbol{r}'} \mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ is bounded everywhere *except* at $\boldsymbol{r} = \boldsymbol{r}'$. Thus, for $\boldsymbol{r} \approx \boldsymbol{r}'$ the *most dominant* contribution to $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ is obtained by the approximate differential equation (*cf.* Eq. (F6))

$$
\nabla^2_{\boldsymbol{r}} \nabla^2_{\boldsymbol{r}'} \mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}') \approx \big(e^2/\epsilon_0\big)^2\, n(\boldsymbol{r})\, \delta(\boldsymbol{r} - \boldsymbol{r}'). \qquad \text{(F7)}
$$

It is readily verified that this equation has the following solution

$$
\begin{aligned}
\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}') &\approx \mathcal{A}'_0 - \frac{n_0 e^4}{8\pi\epsilon_0^2} \|\boldsymbol{r} - \boldsymbol{r}'\| \\
&\quad + \int \mathrm{d}^3 r''\; \mathrm{e}^{-\kappa\|\boldsymbol{r} - \boldsymbol{r}''\|}\, \mathrm{e}^{-\kappa\|\boldsymbol{r}' - \boldsymbol{r}''\|} \\
&\quad\quad \times v_c(\boldsymbol{r} - \boldsymbol{r}'') v_c(\boldsymbol{r}' - \boldsymbol{r}'')\, n'(\boldsymbol{r}''), \qquad \text{(F8)}
\end{aligned}
$$

[125] Note that $\Gamma^{(2)}(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma'; \boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') \equiv n_0^2\, \mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r}, \boldsymbol{r}')$ (see Eq. (B21)).

which is demonstrably *bounded* (for $n'(\boldsymbol{r}'')$ see Eq. (12); note that for uniform GSs, $n' \equiv 0$). Here $\mathcal{A}'_0$ is a constant. We point out that similar to the *exact* $\mathcal{A}'(\boldsymbol{r},\boldsymbol{r}')$, this approximate solution (which has a 'cusp'-like behaviour) is symmetric with respect to the exchange $\boldsymbol{r} \rightleftharpoons \boldsymbol{r}'$.

b. Uniform and isotropic systems

We now complement our above general considerations by directly dealing with $\mathcal{A}'(\boldsymbol{r},\boldsymbol{r}')$ pertaining to uniform and isotropic systems, giving especial attention to $\mathcal{A}'(\boldsymbol{r},\boldsymbol{r}')$ within the framework of the SSDA (see Appendix C). As we shall see, these considerations directly lead us to deduce the functional form of $\mathcal{A}'^{\rm h}(\|\boldsymbol{r}\| = 0)$ pertaining to the fully *interacting* system. For clarity, here as elsewhere in this paper we employ the notation

$$F^{\rm h}(\|\boldsymbol{r}-\boldsymbol{r}'\|) \equiv F(\boldsymbol{r},\boldsymbol{r}') \tag{F9}$$

when dealing with two-point functions pertaining to uniform and isotropic GSs. The following analyses will in addition demonstrate the hazards of inappropriately neglecting the soft cut-off function $\exp(-\kappa\|\boldsymbol{r}-\boldsymbol{r}'\|)$ with which $v(\boldsymbol{r}-\boldsymbol{r}')$ has to be multiplied when $v \equiv v_c$ (*cf.* Eq. (13)). We note that $\mathcal{A}'^{\rm h}(0)$ is the same quantity as $\mathcal{A}'_0$ in Eq. (F8) (recall that here $n' \equiv 0$) and that, for uniform GSs, it *fully* determines the *local* part of $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ (*cf.* Eq. (187)); for *non*-uniform systems, on the other hand, $\Sigma^{\rm l}_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ is fully determined by the $\boldsymbol{r}$-dependent function $\mathcal{A}'(\boldsymbol{r},\boldsymbol{r})$.

Making use of Eq. (B1), while employing (see Appendix C)

$$\Gamma^{(2)}_{\rm s}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') = n_{{\rm s};\sigma}(\boldsymbol{r}) n_{{\rm s};\sigma'}(\boldsymbol{r}') - \delta_{\sigma,\sigma'}\varrho^2_{{\rm s};\sigma}(\boldsymbol{r}',\boldsymbol{r}), \tag{F10}$$

from Eq. (F4) we obtain

$$\mathcal{U}_{\rm s}(\boldsymbol{r}''_1,\boldsymbol{r}''_2) = n_{\rm s}(\boldsymbol{r}''_1)\,\delta(\boldsymbol{r}''_1-\boldsymbol{r}''_2) - \sum_{\sigma'} \varrho^2_{{\rm s};\sigma'}(\boldsymbol{r}''_2,\boldsymbol{r}''_1). \tag{F11}$$

Here as elsewhere in the present work, $\varrho_{{\rm s};\sigma}$ denotes the single-particle Slater-Fock density matrix and $n_{\rm s}$ the *total* number density pertaining to the SSDA of the GS of the system; the use in Eq. (F11) of the interacting density matrix ϱ_σ (rather than $\varrho_{{\rm s};\sigma}$) gives rise to violation of the exact results in Eq. (F5) (irrespective of whether in Eq. (F11) $n_{\rm s}$ is maintained *or* replaced by its exact counterpart n), this owing to the *non*-idempotency of the interacting density matrix (see Appendix C).

For later reference, we re-write the result in Eq. (F4) in the following appealing form (*cf.* Eq. (F11))

$$\mathcal{U}(\boldsymbol{r}''_1,\boldsymbol{r}''_2) = n(\boldsymbol{r}''_1)\,\delta(\boldsymbol{r}''_1-\boldsymbol{r}''_2) - \rho(\boldsymbol{r}''_2,\boldsymbol{r}''_1), \tag{F12}$$

where

$$\rho(\boldsymbol{r}''_2,\boldsymbol{r}''_1) := n(\boldsymbol{r}''_1) n(\boldsymbol{r}''_2) - \sum_{\sigma'_1,\sigma'_2} \Gamma^{(2)}(\boldsymbol{r}''_1\sigma'_1,\boldsymbol{r}''_2\sigma'_2;\boldsymbol{r}''_1\sigma'_1,\boldsymbol{r}''_2\sigma'_2). \tag{F13}$$

Evidently, similar to $\sum_{\sigma'} \varrho^2_{{\rm s};\sigma'}(\boldsymbol{r}''_2,\boldsymbol{r}''_1) \equiv \rho_{\rm s}(\boldsymbol{r}''_2,\boldsymbol{r}''_1)$ on the RHS of Eq. (F11), $\rho(\boldsymbol{r}''_2,\boldsymbol{r}''_1)$ is symmetric with respect to the operation $\boldsymbol{r}''_1 \rightleftharpoons \boldsymbol{r}''_2$. Further, making use of the contraction formula in Eq. (B11), one can readily show that

$$\int {\rm d}^d r''_2\; \rho(\boldsymbol{r}''_2,\boldsymbol{r}''_1) = n(\boldsymbol{r}''_1), \tag{F14}$$

which guarantees satisfaction of the conditions in Eq. (F5). It is interesting to note that, owing to the idempotency of $\varrho_{{\rm s};\sigma}(\boldsymbol{r}''_2,\boldsymbol{r}''_1)$ (*cf.* Eq. (166)), we similarly have

$$\int {\rm d}^d r''_2\; \sum_{\sigma'} \varrho^2_{{\rm s};\sigma'}(\boldsymbol{r}''_2,\boldsymbol{r}''_1) = n_{\rm s}(\boldsymbol{r}''_1). \tag{F15}$$

For uniform GSs, $n_{\rm s}$ coincides with n_0, the total concentration of particles (see Eq. (9)), and is therefore independent of interaction. For non-uniform GSs, on the other hand, in general $n_{\rm s}(\boldsymbol{r}) \not\equiv n(\boldsymbol{r})$, however under the conditions that we have specified in § III.C (see the paragraph that includes Eqs. (54) and (55)), it *is* in general possible to choose the 'non-interacting' Hamiltonian $\widehat{H}_0$ such that the corresponding GS number density $n_{\rm s}(\boldsymbol{r})$ identically coincides with $n(\boldsymbol{r})$. By choosing the Slater determinant employed within the framework of the SSDA to be the GS of such an $\widehat{H}_0$, not only do the first terms on the RHSs of Eqs. (F11) and (F12) become identical, but also the integrals of the second terms yield identical results, as evidenced by Eqs. (F14) and (F15) (see footnote 7 and the associated text in § I.B). Finally, for uniform GSs where $n(\boldsymbol{r}''_1)n(\boldsymbol{r}''_2) = n_0^2$ (see Eq. (12)), $\rho(\boldsymbol{r}''_2,\boldsymbol{r}''_1)$ in Eq. (F13) correctly reduces to a function of $\boldsymbol{r}''_1 - \boldsymbol{r}''_2$. In what follows, we concentrate on systems with uniform *and* isotropic GSs and consequently where appropriate, denote $\varrho_{{\rm s};\sigma'}(\boldsymbol{r}''_2,\boldsymbol{r}''_1)$ and $\rho(\boldsymbol{r}''_2,\boldsymbol{r}''_1)$ by $\varrho^{\rm h}_{{\rm s};\sigma'}(\|\boldsymbol{r}''_2-\boldsymbol{r}''_1\|)$ and $\rho^{\rm h}(\|\boldsymbol{r}''_2-\boldsymbol{r}''_1\|)$, respectively (see Eq. (F9) above).

Substitution of the RHS of Eq. (F12) into that of Eq. (F3), followed by two consequent transformations of variables, yields

$$\mathcal{A}'^{\rm h}(\|\tilde{\boldsymbol{r}}\|) = \int {\rm d}^3 r''\; v_c(\boldsymbol{r}'') \Big[n_0\, \exp(-\kappa\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|) \times v_c(\tilde{\boldsymbol{r}}-\boldsymbol{r}'') - \mathcal{I}_\kappa(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')\Big], \tag{F16}$$

where $\tilde{\boldsymbol{r}} := \boldsymbol{r}-\boldsymbol{r}'$ and

$$\mathcal{I}_\kappa(\boldsymbol{r}) := \int {\rm d}^3 r''\; \exp(-\kappa\|\boldsymbol{r}-\boldsymbol{r}''\|)\, v_c(\boldsymbol{r}-\boldsymbol{r}'')\, \rho^{\rm h}(\|\boldsymbol{r}''\|). \tag{F17}$$

The expression for $\mathcal{A}'^{\mathrm{h}}_{\mathrm{s}}(\|\tilde{\boldsymbol{r}}\|)$ is directly deduced from that in Eq. (F16) through replacing $\mathcal{I}_\kappa(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')$ herein by $\mathcal{I}_{\mathrm{s};\kappa}(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')$, where

$$\mathcal{I}_{\mathrm{s};\kappa}(\boldsymbol{r}) \equiv \mathcal{I}_\kappa(\boldsymbol{r})\vert_{\rho^{\mathrm{h}}\rightharpoonup \sum_{\sigma'}(\varrho^{\mathrm{h}}_{\mathrm{s};\sigma'})^2}\,. \tag{F18}$$

In order to investigate the behaviour of $\mathcal{A}'^{\mathrm{h}}_{\mathrm{s}}(\|\tilde{\boldsymbol{r}}\|)$, we first consider $\mathcal{I}_{\mathrm{s};\kappa}(\boldsymbol{r})$ in Eq. (F18), with $\mathcal{I}_\kappa(\boldsymbol{r})$ herein defined according to Eq. (F17). Since $\varrho^{\mathrm{h}}_{\mathrm{s};\sigma'}(\|\boldsymbol{r}''\|)$ is bounded everywhere, the possibility that $\mathcal{I}_{\mathrm{s};\kappa}(\boldsymbol{r})$ be unbounded solely depends on the possibility of a slow decay of the integrand in the defining expression for $\mathcal{I}_{\mathrm{s};\kappa}(\boldsymbol{r})$ as $\|\boldsymbol{r}''\|\to\infty$. Later in this Appendix we shall see that (*cf.* Eq. (F24) below; see also Appendix J)

$$\varrho^{\mathrm{h}}_{\mathrm{s};\sigma}(\|\boldsymbol{r}''\|) \sim \frac{-k_{F;\sigma}}{2\pi^2}\,\frac{\cos(k_{F;\sigma}\|\boldsymbol{r}''\|)}{\|\boldsymbol{r}''\|^2},\quad \|\boldsymbol{r}''\|\to\infty, \tag{F19}$$

where $k_{F;\sigma}$ stands for the Fermi wavenumber of the fermions with spin σ (here we are assuming that $N_\sigma \neq 0$). The result in Eq. (F19) applies also to the density matrix pertaining to the fully *interacting* uniform and isotropic GS, with the provision that the RHS of Eq. (F19) be multiplied by $Z_{F;\sigma}$ (Farid 2000a — see also Appendix J), the amount of jump in the momentum distribution function $\mathsf{n}_\sigma(\boldsymbol{k})$ at $k_{F;\sigma}$ (for definition see Eq. (J2) below); here we make the implicit assumption that the interacting GS is uniform and metallic, and moreover the corresponding Fermi seas are spherical in shape. For completeness, we mention the important fact that in cases where $Z_{F;\sigma}=0$ (for *some* σ), the leading-order term in the large-$\|\boldsymbol{r}\|$ AS for $\varrho^{\mathrm{h}}_\sigma(\|\boldsymbol{r}\|)$ is fundamentally different in comparison with that on the RHS of Eq. (F19); in the case of $Z_{F;\sigma}=0$, $\varrho^{\mathrm{h}}_\sigma(\|\tilde{\boldsymbol{r}}\|)$ to leading order decays in magnitude like $1/\|\tilde{\boldsymbol{r}}\|^{2+\alpha}$ (when $d=3$), where $\alpha>0$ is referred to as the *anomalous exponent*. We note in passing that the property $Z_{F;\sigma}<1$ reflects the *non*-idempotency of $\varrho^{\mathrm{h}}_\sigma(\|\tilde{\boldsymbol{r}}\|)$ which in turn is a manifestation of the over-completeness of the set of the Lehmann amplitudes (see Appendix A).

From the result in Eq. (F19), it follows that for $\|\boldsymbol{r}''\|\to\infty$, barring the exponential cut-off function, the integrand on the RHS of Eq. (F17), with ρ^{h} herein replaced by $\sum_\sigma(\varrho_{\mathrm{s};\sigma})^2$ (see Eq. (F18)), *decays* like $1/\|\boldsymbol{r}''\|^5$ which is sufficient for the existence of $\mathcal{I}_{\mathrm{s};\kappa}(\boldsymbol{r})$ with $\kappa=0$: with $\mathrm{d}^3r''=\mathrm{d}\varphi\,\mathrm{d}\theta\,\mathrm{d}r''\,r''^2\sin(\theta)$ in the spherical-polar coordinates system, it is seen that the integrand in the radial direction *decays* like $1/r''^3$ for $r''\to\infty$; consequently, $\mathcal{I}_{\mathrm{s};\kappa=0}(\boldsymbol{r}) \equiv \lim_{\kappa\downarrow 0}\mathcal{I}_{\mathrm{s};\kappa}(\boldsymbol{r})$. As we shall see, this fact notwithstanding, identifying κ in Eq. (F16) with zero *prior to* evaluating $\mathcal{A}'^{\mathrm{h}}_{\mathrm{s}}(\|\boldsymbol{r}\|=0)$, gives rise to an erroneous outcome in the case at hand.

We now proceed with considering $\mathcal{A}'^{\mathrm{h}}_{\mathrm{s}}(\|\tilde{\boldsymbol{r}}\|)$ by investigating the behaviour of the integrand of the $\boldsymbol{r}''$ integral on the RHS of Eq. (F16). Since, following our above discussion, $\mathcal{I}_{\mathrm{s};\kappa}(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')$ is bounded for *all* $\boldsymbol{r}''$, and since the singularities of $v_c(\boldsymbol{r}'')$ and $v_c(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')$ at $\boldsymbol{r}''=\boldsymbol{0}$ and $\boldsymbol{r}''=\tilde{\boldsymbol{r}}$ respectively are integrable, the boundedness or otherwise of $\mathcal{A}'^{\mathrm{h}}_{\mathrm{s}}(\|\tilde{\boldsymbol{r}}\|)$ is entirely determined by the behaviour of the integrand of the $\boldsymbol{r}''$ integral for $\|\boldsymbol{r}''\|\to\infty$. In order to establish this behaviour, we need to determine that of $\mathcal{I}_{\mathrm{s};\kappa}(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')$ in the asymptotic region $\|\boldsymbol{r}''\|\to\infty$, which for finite $\|\tilde{\boldsymbol{r}}\|$ corresponds to $\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|\to\infty$. To this end, we employ the multipole expansion (for example Jackson (1975) or Morse and Feshbach (1953)) (below $\widehat{\boldsymbol{r}}{:=}\boldsymbol{r}/\|\boldsymbol{r}\|$)

$$v_c(\boldsymbol{r}-\boldsymbol{r}'') = v_c(\boldsymbol{r}) + \frac{v_c(\boldsymbol{r})\,\widehat{\boldsymbol{r}}\cdot\boldsymbol{r}''}{\|\boldsymbol{r}\|} + \mathcal{O}\big(1/\|\boldsymbol{r}\|^3\big) \tag{F20}$$

in the regime of $\|\boldsymbol{r}\|\to\infty$ (which for finite values of $\|\boldsymbol{r}''\|$, corresponds to $\|\boldsymbol{r}-\boldsymbol{r}''\|\to\infty$). From this, making use of Eq. (F14), for $\mathcal{I}_\kappa(\boldsymbol{r})$ in Eq. (F17) we readily obtain the following leading-order result:

$$\mathcal{I}_\kappa(\boldsymbol{r}) \sim \exp(-\kappa\|\boldsymbol{r}\|)\,n_0\,v_c(\boldsymbol{r}),\quad \|\boldsymbol{r}\|\to\infty; \tag{F21}$$

since n_0 is independent of interaction, the RHS of Eq. (F21) equally applies to $\mathcal{I}_{\mathrm{s};\kappa}(\boldsymbol{r})$. In light of Eq. (F21), for $\|\boldsymbol{r}''\|\to\infty$ (or $\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|\to\infty$ when $\|\tilde{\boldsymbol{r}}\|<\infty$), the *leading* term in the AS of the integrand of the $\boldsymbol{r}''$ integral on the RHS of Eq. (F16) is determined by the *next-to-leading* term in the AS of $\mathcal{I}_\kappa(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')$. Due to the isotropy of $\rho^{\mathrm{h}}(\|\boldsymbol{r}''\|)$,

$$\int \mathrm{d}^3r''\;\mathrm{e}^{-\kappa\|\boldsymbol{r}-\boldsymbol{r}''\|}\,\hat{\boldsymbol{r}}\cdot\boldsymbol{r}''\,\rho^{\mathrm{h}}(\|\boldsymbol{r}''\|)\equiv 0,\quad \kappa\downarrow 0, \tag{F22}$$

so that the term in the indicated large-$\|\boldsymbol{r}''\|$ AS for $\mathcal{I}_\kappa(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')$, which according to Eq. (F20) would decay like $v_c(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')/\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|$, is vanishing. The absence of a terms decaying like

$$\frac{v_c(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')}{\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|} \propto \frac{1}{\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|^2}$$

in the large-$\|\boldsymbol{r}''\|$ AS of $\mathcal{I}_\kappa(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')$ (or $\mathcal{I}_{\mathrm{s};\kappa}(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')$) implies that the term enclosed by the square brackets on the RHS of Eq. (F16) decays *more rapidly* [126] than $1/\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|^2$. As we shall see shortly, this aspect, which is of vital consequence for the boundedness of $\mathcal{A}'^{\mathrm{h}}_{\mathrm{s}}(0)$ in the limit $\kappa\downarrow 0$, is *not* accounted for by the expression for $\mathcal{I}_{\mathrm{s};\kappa=0}(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')$ (or $\mathcal{I}_{\kappa=0}(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')$). It should be mentioned that, through identifying κ with zero *prior to* carrying out the $\boldsymbol{r}''$ integral on the LHS of Eq. (F22), this integral would become

[126] A note of caution is in place here; contrary to the considerations related to the AS expansions of functions of ε (or of z), for $|\varepsilon|\to\infty$ (or $|z|\to\infty$) considered in this paper, here the Poincaré definition of AS (see § II.B) is restrictive (we have some circumstantial evidence indicating this to be the case). See footnote 28.

ill-defined, rendering the result in Eq. (F22) only conditionally valid; to deduce Eq. (F22) (while $\kappa = 0$), it is required that, in evaluating the $\boldsymbol{r}''$ integral in terms of the spherical polar coordinates of $\boldsymbol{r}''$, that is (r'', θ, φ), the integration with respect to $\varphi \in [0, 2\pi)$ be carried out *prior to* that with respect to $r'' \in [0, R)$, $R = \infty$; with $\kappa = 0$, in view of the asymptotic result to be presented in Eqs. (F69) and (F101) below, the latter integral can be shown to diverge like $\sum_{\sigma'} \ln(k_{F;\sigma'} R)$ as $R \to \infty$ (see § II.A and the text following Eq. (10)).

Since, in the limit $\kappa \downarrow 0$, the contribution corresponding to the third term in the multipole expansion of $v_c(\boldsymbol{r} - \boldsymbol{r}'')$ gives rise to an unbounded $\boldsymbol{r}''$ integral on the RHS of Eq. (F17), we deduce that the *next-to-leading* term in the large-$\|\boldsymbol{r}\|$ AS for $\mathcal{I}_\kappa(\boldsymbol{r})$ (or $\mathcal{I}_{\mathrm{s};\kappa}(\boldsymbol{r})$) *cannot* be one decaying like $1/\|\boldsymbol{r}\|^3$, but a term decaying more slowly; however, it decays more rapidly than (see footnote 126) $1/\|\boldsymbol{r}\|^2$. This implies that $\mathcal{A}'^{\mathrm{h}}(\|\tilde{\boldsymbol{r}}\|)$ (or $\mathcal{A}_{\mathrm{s}}'^{\mathrm{h}}(\|\tilde{\boldsymbol{r}}\|)$) in Eq. (F16) is indeed a bounded function for *all* $\tilde{\boldsymbol{r}}$, in full conformity with our finding based on general considerations (see Eq. (F8) above and the text following it; see also Eq. (F59) below and the succeeding text as well as footnote 129).

We now consider the crucial role played by a non-vanishing κ in rendering the expression in Eq. (F16) well defined. To this end we first recall that, for non-interacting uniform systems, we have (see Eqs. (46) and (47))

$$f_{s;\sigma}(\boldsymbol{r}) \Longrightarrow \phi_{\boldsymbol{k}}(\boldsymbol{r}) \equiv \frac{1}{\Omega^{1/2}} \exp(i\boldsymbol{k}\cdot\boldsymbol{r}), \tag{F23}$$

so that for uniform and isotropic GSs (the attribute 'isotropic' is reflected in the condition $\|\boldsymbol{k}\| \le k_{F;\sigma}$ invoked below) (see Eq. (169)) (March, *et al.* 1967, pp. 15 and 16),

$$\begin{aligned}\varrho_{\mathrm{s};\sigma}^{\mathrm{h}}(\|\boldsymbol{r}-\boldsymbol{r}'\|) &= \frac{1}{\Omega} \sum_{\|\boldsymbol{k}\| \le k_{F;\sigma}} \exp(-i\boldsymbol{k}\cdot[\boldsymbol{r}-\boldsymbol{r}'])\\ &= \frac{1}{(2\pi)^3} \int_{\|\boldsymbol{k}\| \le k_{F;\sigma}} \mathrm{d}^3k\, \exp(-i\boldsymbol{k}\cdot[\boldsymbol{r}-\boldsymbol{r}'])\\ &= \frac{k_{F;\sigma}^2}{2\pi^2}\, \frac{j_1\big(k_{F;\sigma}\|\boldsymbol{r}-\boldsymbol{r}'\|\big)}{\|\boldsymbol{r}-\boldsymbol{r}'\|},\end{aligned} \tag{F24}$$

where $j_1(x)$ stands for the spherical Bessel function of the first order, defined as (Abramowitz and Stegun 1972, p. 438)

$$j_1(x) := \frac{\sin(x) - x\cos(x)}{x^2}. \tag{F25}$$

The asymptotic result in Eq. (F19) is trivially deduced from the expression in Eq. (F24) through making use of $j_1(x) \sim -\cos(x)/x$ for $|x| \to \infty$.

From Eqs. (F11) and (F24) and employing $n_{0;\sigma} = k_{F;\sigma}^3/[6\pi^2]$, we obtain

$$\mathcal{U}_{\mathrm{s}}(\boldsymbol{r},\boldsymbol{r}') = n_0\delta(\boldsymbol{r}-\boldsymbol{r}') - \sum_{\sigma'} \frac{9n_{0;\sigma'}^2}{k_{F;\sigma'}^2}\, \frac{j_1^2(k_{F;\sigma'}\|\boldsymbol{r}-\boldsymbol{r}'\|)}{\|\boldsymbol{r}-\boldsymbol{r}'\|^2}. \tag{F26}$$

From now onwards we assume $n_{0;\sigma} = n_{0;\bar{\sigma}} = n_0/2$ (corresponding to uniform and isotropic systems of spin-1/2 fermions, i.e. $\mathsf{s} = 1/2$, in the paramagnetic state) and thus $k_{F;\sigma} = k_{F;\bar{\sigma}} = k_F = (3\pi^2 n_0)^{1/3}$.

Employing the Fourier representation of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ (see Eq. (G2)), from Eqs. (F17), (F18) and (F24) we obtain

$$\begin{aligned}\mathcal{I}_{\mathrm{s};\kappa=0}(\tilde{\boldsymbol{r}}-\boldsymbol{r}'') &= \frac{9n_0^2}{2k_F^2} \int \mathrm{d}^3 r_1''\; v_c(\tilde{\boldsymbol{r}}-\boldsymbol{r}_1'')\\ &\qquad\times \frac{j_1^2(k_F\|\boldsymbol{r}''-\boldsymbol{r}_1''\|)}{\|\boldsymbol{r}''-\boldsymbol{r}_1''\|^2}\\ &= \frac{9n_0^2}{2k_F^2} \int \frac{\mathrm{d}^3 q}{(2\pi)^3}\, \frac{e^2/\epsilon_0}{\|\boldsymbol{q}\|^2}\, \mathrm{e}^{i\boldsymbol{q}\cdot(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')}\\ &\qquad\times \frac{4\pi}{\|\boldsymbol{q}\|} \int_0^\infty \mathrm{d}r_1''\, \frac{j_1^2(k_F r_1'')\,\sin(\|\boldsymbol{q}\| r_1'')}{r_1''}.\end{aligned} \tag{F27}$$

With $\|\boldsymbol{q}\| > 0$, we have the standard result

$$\begin{aligned}\int_0^\infty \mathrm{d}r_1''\, \frac{j_1^2(k_F r_1'')\,\sin(\|\boldsymbol{q}\| r_1'')}{r_1''} &= \frac{\pi\|\boldsymbol{q}\|}{96 k_F^4}\,(2k_F - \|\boldsymbol{q}\|)^2\\ &\qquad\times(4k_F + \|\boldsymbol{q}\|)\,\Theta(2k_F - \|\boldsymbol{q}\|),\end{aligned} \tag{F28}$$

substitution of which into the RHS of Eq. (F27) yields [127]

$$\begin{aligned}\mathcal{I}_{\mathrm{s};\kappa=0}(\tilde{\boldsymbol{r}}-\boldsymbol{r}'') &= \frac{n_0}{4\pi k_F^3}\, v_c(\tilde{\boldsymbol{r}}-\boldsymbol{r}'')\, \frac{1}{\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|^3}\\ &\times\Big\{ -1 - 6k_F^2\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|^2\\ &\quad + \big(1 + 4k_F^2\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|^2\big)\,\cos(2k_F\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|)\\ &\quad + 2k_F\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|\sin(2k_F\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|)\\ &\quad + 8k_F^3\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|^3\,\mathrm{Si}(2k_F\|\tilde{\boldsymbol{r}}-\boldsymbol{r}''\|)\Big\},\end{aligned} \tag{F29}$$

where $\mathrm{Si}(x)$ stands for the sine-integral function (Abramowitz and Stegun 1972, p. 231). The linearity with respect to $\|\boldsymbol{q}\|$ of the expression on the RHS of Eq. (F28) for small values of $\|\boldsymbol{q}\|$ (to leading order, one has $\pi\|\boldsymbol{q}\|/[6k_F]$), as well as the infinitely sharp cut-off $\Theta(2k_F - \|\boldsymbol{q}\|)$ in this expression, are consequences of identifying κ with zero. Below we shall derive the exact expression for $\mathcal{A}_{\mathrm{s}}'^{\mathrm{h}}(0)$ but, before doing so, consider in some detail the undesired consequence to which a premature identification of κ with zero gives rise.

Making use of the asymptotic results $\mathrm{Si}(z) \sim z -$

[127] Recall that $9n_0/[2k_F^2] = 3k_F/[2\pi^2]$.

$z^3/18 + \ldots$, for $|z| \to 0$ and [128] $\mathrm{Si}(z) \sim \pi/2 - \cos(z)/z - \sin(z)/z^2 + \ldots$, for $|z| \to \infty$ ($|\arg(z)| < \pi$) (see Abramowitz and Stegun 1972, pp. 232 and 233), we readily obtain

$$\mathcal{I}_{\mathrm{s};\kappa=0}(\tilde{\boldsymbol{r}} - \boldsymbol{r}'') \sim \frac{e^2}{4\pi\epsilon_0}\,\frac{3k_F n_0}{2\pi^2}, \quad \|\tilde{\boldsymbol{r}} - \boldsymbol{r}''\| \to 0; \quad \text{(F30)}$$

$$\mathcal{I}_{\mathrm{s};\kappa=0}(\tilde{\boldsymbol{r}} - \boldsymbol{r}'') \sim n_0\Big(1 - \frac{3/[2\pi k_F]}{\|\tilde{\boldsymbol{r}} - \boldsymbol{r}''\|} + \ldots\Big)\, v_c(\tilde{\boldsymbol{r}} - \boldsymbol{r}''), \quad \|\tilde{\boldsymbol{r}} - \boldsymbol{r}''\| \to \infty. \quad \text{(F31)}$$

Compare the leading term on the RHS of Eq. (F31) with RHS of Eq. (F21), with κ herein identified with zero. From Eq. (F16) and the results in Eqs. (F30) and (F31), we observe that for $\|\tilde{\boldsymbol{r}} - \boldsymbol{r}''\| \to 0$ the contribution of the terms enclosed by square brackets on the RHS of Eq. (F16) is asymptotically equal to $n_0 v_c(\tilde{\boldsymbol{r}} - \boldsymbol{r}'') \propto 1/\|\tilde{\boldsymbol{r}} - \boldsymbol{r}''\|$, whereas for $\|\tilde{\boldsymbol{r}} - \boldsymbol{r}''\| \to \infty$, the indicated contribution is asymptotically equal to $(3n_0/[2\pi k_F]) v_c(\tilde{\boldsymbol{r}} - \boldsymbol{r}'')/\|\tilde{\boldsymbol{r}} - \boldsymbol{r}''\| \propto 1/\|\tilde{\boldsymbol{r}} - \boldsymbol{r}''\|^2$. This result contradicts our earlier conclusion (see text following Eq. (F22) above), namely that, for $\|\tilde{\boldsymbol{r}} - \boldsymbol{r}''\| \to \infty$, the function enclosed inside the curly braces on the RHS of Eq. (F16) decays *more rapidly* than $1/\|\tilde{\boldsymbol{r}} - \boldsymbol{r}''\|^2$, that is the coefficient of $1/\|\tilde{\boldsymbol{r}} - \boldsymbol{r}''\|^2$ must be identically vanishing.

Now we proceed with the determination of $\mathcal{A}_{\mathrm{s}}'^{\mathrm{h}}(0)$. In doing so, we concentrate on the *exact* $\mathcal{A}'^{\mathrm{h}}(0)$ and only in the final stage explicitly deal with this function within the framework of the SSDA. To this end, we first introduce the pair of Fourier transforms (below $r{:=}\|\boldsymbol{r}\|$ and $q{:=}\|\boldsymbol{q}\|$)

$$\rho^{\mathrm{h}}(r) = \int \frac{\mathrm{d}^3 q}{(2\pi)^3}\, \mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{r}}\, \bar{\rho}^{\mathrm{h}}(q), \quad \text{(F32)}$$

$$\bar{\rho}^{\mathrm{h}}(q) = \int \mathrm{d}^3 r\, \mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\, \rho^{\mathrm{h}}(r), \quad \text{(F33)}$$

from which and Eq. (F17) we readily obtain

$$\mathcal{I}_\kappa(\boldsymbol{r}) = \frac{2}{\pi}\, v_c(\boldsymbol{r}) \int_0^\infty \mathrm{d}q\, \frac{q}{q^2+\kappa^2}\, \bar{\rho}^{\mathrm{h}}(q)\, \sin(qr). \quad \text{(F34)}$$

We note that $\bar{\rho}^{\mathrm{h}}(0) = n_0$ (see Eq. (F14)) and that

$$\int_0^\infty \mathrm{d}x\, \frac{x}{x^2+\kappa^2}\, \sin(ax) = \frac{\pi}{2}\mathrm{sgn}(a)\, \mathrm{e}^{-\kappa a}, \quad \text{(F35)}$$

so that (*cf.* Eq. (F21))

$$\frac{2}{\pi}\, v_c(\boldsymbol{r}) \int_0^\infty \mathrm{d}q\, \frac{q}{q^2+\kappa^2}\, \bar{\rho}^{\mathrm{h}}(0)\, \sin(qr) = \mathrm{e}^{-\kappa r}\, n_0\, v_c(\boldsymbol{r}). \quad \text{(F36)}$$

From this and Eqs. (F16) and (F34) we obtain

$$\mathcal{A}'^{\mathrm{h}}(0) = -\frac{2}{\pi}\int \mathrm{d}^3 r\; v_c^2(\boldsymbol{r})\, \mathrm{e}^{-\kappa r}\, \mathcal{J}_\kappa(r) = -8\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \int_0^\infty \mathrm{d}r\; \mathrm{e}^{-\kappa r}\, \mathcal{J}_\kappa(r), \quad \kappa \downarrow 0, \quad \text{(F37)}$$

where

$$\mathcal{J}_\kappa(r) {:=} \int_0^\infty \mathrm{d}q\, \frac{q\,[\bar{\rho}^{\mathrm{h}}(q) - \bar{\rho}^{\mathrm{h}}(0)]}{q^2+\kappa^2}\, \sin(qr). \quad \text{(F38)}$$

It can be shown that

$$\mathcal{J}_0(r)\vert_{\text{Eq. (F38)}} \sim \frac{\bar{\rho}^{\mathrm{h}\prime}(0)}{r}, \quad \text{for} \quad r \to \infty, \quad \text{(F39)}$$

where $\bar{\rho}^{\mathrm{h}\prime}(0) \equiv \mathrm{d}\bar{\rho}^{\mathrm{h}}(q)/\mathrm{d}q\vert_{q\downarrow 0}$ (concerning the existence of this quantity, see Eqs. (F44) and (F68) below and the subsequent considerations). It follows that $\mathcal{A}'^{\mathrm{h}}(0)$ according to Eq. (F37), with $\mathcal{J}_\kappa(r)$ according to Eq. (F38), diverges like $\ln(\kappa/k_F)$ for $\kappa \downarrow 0$. This divergence has the same origin as discussed above. Below, we construct an expression for $\mathcal{J}_\kappa(r)$ which gives rise to the expected finite value for $\mathcal{A}'^{\mathrm{h}}(0)$ for $\kappa \downarrow 0$.

From Eq. (F33) we readily deduce

$$\bar{\rho}^{\mathrm{h}}(q) - \bar{\rho}^{\mathrm{h}}(0) = 4\pi \int_0^\infty \mathrm{d}r\, r^2\, \rho^{\mathrm{h}}(r)\Big[\frac{\sin(qr)}{qr} - 1\Big]. \quad \text{(F40)}$$

By assuming [129] that $\rho^{\mathrm{h}}(r)$, similar to $\sum_{\sigma'}\big(\varrho^{\mathrm{h}}_{\mathrm{s};\sigma'}(r)\big)^2 \equiv \rho^{\mathrm{h}}_{\mathrm{s}}(r)$, decays like $1/r^4$ for $r \to \infty$ (see Eqs. (F69) and (F101) below), we have

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[128] The *transcendental* functions $\cos(z)$ and $\sin(z)$ encountered in the large-$|z|$ AS of $\mathrm{Si}(z)$ are partly responsible for rendering the Poincaré definition of AS (see § II.B) inadequate in regard to the ensuing functions of spatial coordinates (see footnote 126).

[129] This assumption coincides with fact insofar as $\rho^{\mathrm{h}}_{\mathrm{s}}(r)$ as well as $\rho^{\mathrm{h}}(r)$ pertaining to weakly interacting systems are concerned. As our considerations following Eq. (F68) below show, however, with $\rho^{\mathrm{h}}(r)$ decaying like $1/r^\alpha$ for $r \to \infty$, although it is *not* excluded that $\alpha > 4$, it is strictly excluded that $\alpha < 4$; the latter possibility implies divergence of $\mathcal{A}'^{\mathrm{h}}(0)$ (see Eqs. (F59), (F60), (F61), (F68) and (F55) below) and therefore instability of the GS of the system under consideration. Recall that in states with off-diagonal long-range order (ODLRO) (for definition and some details see, for example, Reichl (1980, pp. 202-205)), including those with *algebraic* ODLRO (here corresponding to cases where $\alpha < 4$; recall that here we are explicitly considering $d = 3$), the *normal* GS assumed here, is indeed not the GS and therefore unstable. In this context, it should be noted that according to Kohn and Luttinger (1965), below a finite, but extremely small, transition temperature, the true GS of a uniform and isotropic system of fermions is *not* normal, but superconducting. It would therefore appear (since we consider the absolute temperature to be zero) that, by using the *true* GS of the system under

$$|\int_0^\infty \mathrm{d}r\, r^\alpha\, \rho^{\rm h}(r)| < \infty \quad \text{for} \quad -1<\alpha<3. \tag{F41}$$

Consequently, from Eq. (F40) we directly deduce that $\bar{\rho}^{\rm h}(q)$ is *continuous* at $q=0$, that is

$$\bar{\rho}^{\rm h}(q) - \bar{\rho}^{\rm h}(0) = o(1) \tag{F42}$$

for $q\in[0,Q]$ with Q some *positive* constant. This is clarified by the observation that on decreasing q towards zero, the minimum value of r beyond which $[\sin(qr)/(qr)-1]$ appreciably deviates from zero increases (by an amount proportional to $1/q$), which, in view of the fact that the integral in Eq. (F41) is bounded for $\alpha=2$, through Eq. (F40) results in Eq. (F41). The condition in Eq. (F41) is weaker than that in which $o(1)$ on the RHS of Eq. (F42) is replaced by $\mathcal{O}(q)$, implying $\bar{\rho}^{\rm h}(q)$ to be a (right) *differentiable* function of q in $[0,Q]$ (see text following Eq. (F44) below). By employing $\sin(x)/x\sim 1-x^2/6$, for $x\to 0$, in the RHS of Eq. (F40), we further deduce that $o(1)$ on the RHS of Eq. (F42) *cannot* be equal to $\mathcal{O}(q^2)$ but to some function which for $q\downarrow 0$ is more dominant than $\mathcal{O}(q^2)$ (but, by continuity, less dominant than $o(1)$; see above). This follows from the fact that the integral in Eq. (F41) is divergent for $\alpha=4$ (see the considerations in § II.B). Our calculations, to be presented below, combined with our above observations, lead us to the conclusion that in addition to being *continuous*, $\bar{\rho}^{\rm h}(q)$ is a *continuously differentiable* function of q for $q\in[0,Q]$ with $Q>0$, i.e.

$$\bar{\rho}^{\rm h}(q) = \bar{\rho}^{\rm h}(0) + \bar{\rho}^{\rm h\prime}(0)\, q + o(q), \quad \text{where } \textit{possibly}\;\; q^2/o(q)\to 0 \;\text{ as }\; q\downarrow 0; \tag{F43}$$

for $\bar{\rho}^{\rm h}_{\rm s}(q)$, the above $o(q)$ is equal to $\mathcal{O}(q^3)$, however. For later reference, from Eq. (F40) we have

$$\bar{\rho}^{\rm h\prime}(q) := \frac{\mathrm{d}\bar{\rho}^{\rm h}(q)}{\mathrm{d}q} = \frac{4\pi}{q}\int_0^\infty \mathrm{d}r\, r^2\, \rho^{\rm h}(r)\Big[\cos(qr) - \frac{\sin(qr)}{qr}\Big]. \tag{F44}$$

We point out that since by definition $q\ge 0$, in Eq. (F43) as well as below, $\bar{\rho}^{\rm h\prime}(0)$ should be considered as denoting the *right*-derivative of $\bar{\rho}^{\rm h}(q)$ with respect to q at $q=0$. Later we investigate the condition for the boundedness of $\bar{\rho}^{\rm h\prime}(0)$ is some detail (see the paragraph containing Eq. (F68) below).

From the expression in Eq. (F40), through repeated application of integration by parts (compare with a similar procedure adopted in Appendix J) and making use of the Riemann-Lebesgue lemma (Whittaker and Watson 1927, p. 172) we deduce (below $\rho^{\rm h\prime}(0) := \mathrm{d}\rho^{\rm h}(r)/\mathrm{d}r|_{r\downarrow 0}$; we note that $\rho^{\rm h\prime}_{\rm s}(0)=0$)

$$\bar{\rho}^{\rm h}(q) \sim -8\pi\, \frac{\rho^{\rm h\prime}(0)}{q^4} \quad \text{for} \quad q\to\infty, \tag{F45}$$

so that through integration by parts, from Eq. (F38) we obtain

$$\mathcal{J}_\kappa(r) = \frac{1}{r}\int_0^\infty \mathrm{d}q\, \Big[\frac{\mathrm{d}}{\mathrm{d}q}\, \frac{q\,[\bar{\rho}^{\rm h}(q)-\bar{\rho}^{\rm h}(0)]}{q^2+\kappa^2}\Big]\, \cos(qr), \tag{F46}$$

to which no boundary terms have contributed, for

$$\frac{-1}{r}\, \cos(qr)\, \frac{q\,[\bar{\rho}^{\rm h}(q)-\bar{\rho}^{\rm h}(0)]}{q^2+\kappa^2}\Big|_{q=0}^{\infty} = 0. \tag{F47}$$

It is here that a finite κ, even though infinitesimally small, manifests its essential role; from Eq. (F47) we observe that with $\kappa=0$ (as opposed to $\kappa\downarrow 0$), the LHS of Eq. (F47) would have been equal to $\mathcal{O}(1/r)$ (to be precise, in view of Eq. (F43), equal to $\bar{\rho}^{\rm h\prime}(0)/r$) arising from the $q=0$ side of the integration boundary, rather than zero as in Eq. (F47). This non-vanishing contribution of order $1/r$ is directly related to the second term inside the large parentheses on the RHS of Eq. (F31) resulting from a premature identification of κ with zero; in this connection note that $-n_0\times 3/[2\pi k_F]$ encountered on the RHS of Eq. (F31) is exactly equal to $(2/\pi)\times\bar{\rho}^{\rm h\prime}_{\rm s}(0)$, where $\bar{\rho}^{\rm h\prime}_{\rm s}(0) = -k_F^2/[4\pi^2] \equiv -3n_0/[4k_F]$ and where $2/\pi$ originates from the RHS of Eq. (F34).

Making use of $[\bar{\rho}^{\rm h}(q)-\bar{\rho}^{\rm h}(0)]/q = \bar{\rho}^{\rm h\prime}(0)+o(1)$ and $\bar{\rho}^{\rm h\prime}(q)-\bar{\rho}^{\rm h\prime}(0) = o(1)$, for $q\to 0$, both of which follow from Eq. (F43), we have

$$\frac{\mathrm{d}}{\mathrm{d}q}\, \frac{q\,[\bar{\rho}^{\rm h}(q)-\bar{\rho}^{\rm h}(0)]}{q^2+\kappa^2}\Big|_{\kappa=0} \equiv \frac{\bar{\rho}^{\rm h\prime}(q) - [\bar{\rho}^{\rm h}(q)-\bar{\rho}^{\rm h}(0)]/q}{q} = o(1/q) \quad \text{for} \quad q\to 0. \tag{F48}$$

From this we conclude that for $\kappa=0$, the integrand of the q integral on the RHS of Eq. (F46) is integrable in the neighbourhood of $q=0$. Further, from Eq. (F45) we have (for considerations related to derivatives of AS and AS of derivatives see, for example, Lauwerier (1977)) $\bar{\rho}^{\rm h\prime}(q)\sim 32\pi\rho^{\rm h\prime}(0)/q^5$ for $q\to\infty$ so that, for $q\to\infty$ the integrand of the integral on the RHS of Eq. (F46), as enclosed by square brackets, behaves like $\bar{\rho}^{\rm h}(0)/q^2$. We thus conclude that $\mathcal{J}_\kappa(r)$ according to Eq. (F46) is a well-defined function of r for $\kappa=0$.

On account of the Riemann-Lebesgue lemma (Whittaker and Watson 1927, p. 172) we have

consideration, we should expect $\mathcal{A}'^{\rm h}(0)$ to be unbounded. Use of such a GS, however, is *not* justified within the framework of our present work, where by assumption the GS of the system is *normal*; in order to be able to deal with systems with, say, superconducting GSs, we should have utilized the Nambu (1960) formalism (Fetter and Walecka 1971, p. 443), thus taking account of the possibility of a non-vanishing *anomalous* GF, signifying ODLRO in the system.

$$\int_0^\infty \mathrm{d}q\, \Big[\frac{\mathrm{d}}{\mathrm{d}q} \frac{q\,[\bar{\rho}^{\mathrm{h}}(q)-\bar{\rho}^{\mathrm{h}}(0)]}{q^2+\kappa^2}\Big] \cos(qr) = o(1) \;\text{ for }\; r\to\infty, \tag{F49}$$

so that $\mathscr{J}_\kappa(r)$ as presented in Eq. (F46) decays *faster* than $1/r$ for $r\to\infty$. The behaviour $\mathscr{J}_\kappa(r)=o(1/r)$ (to be contrasted with $\mathcal{O}(1/r)$ discussed above) for $r\to\infty$, exactly reflects the property that we have earlier deduced through employing the multipole expansion in Eq. (F20) in our investigation of the large-$\|\boldsymbol{r}\|$ asymptotic behaviour of $\mathcal{I}_\kappa(\boldsymbol{r})$, culminating in Eq. (F22) and the subsequent conclusions. In spite of this desired property of the $\mathscr{J}_\kappa(r)$ in Eq. (F46) as $r\to\infty$, for $\kappa=0$ this function can be shown to behave like (*cf.* Eq. (F39) above)

$$\mathscr{J}_0(r)\vert_{\text{Eq. (F46)}} \sim -\frac{\bar{\rho}^{\mathrm{h}\prime}(0)}{r}, \quad \text{for} \quad r\to 0. \tag{F50}$$

It follows that $\mathcal{A}'^{\mathrm{h}}(0)$ according to Eq. (F37) with $\mathscr{J}_\kappa(r)$ as presented in Eq. (F46) also diverges like $\ln(\kappa/k_F)$ for $\kappa\downarrow 0$. Thus $\mathscr{J}_\kappa(r)$ neither according to Eq. (F38) nor according to Eq. (F46) is the appropriate function for calculating $\mathcal{A}'^{\mathrm{h}}(0)$.

The equivalence of the expressions in Eqs. (F38) and (F46) for $\kappa>0$ implies that for $\kappa>0$ we can define $\mathscr{J}_\kappa(r)$ as follows

$$\mathscr{J}_\kappa(r) := \frac{1}{2}\Big\{\int_0^\infty \mathrm{d}q\, \frac{q\,[\bar{\rho}^{\mathrm{h}}(q)-\bar{\rho}^{\mathrm{h}}(0)]}{q^2+\kappa^2}\, \sin(qr) + \frac{1}{r}\int_0^\infty \mathrm{d}q\, \Big[\frac{\mathrm{d}}{\mathrm{d}q}\frac{q\,[\bar{\rho}^{\mathrm{h}}(q)-\bar{\rho}^{\mathrm{h}}(0)]}{q^2+\kappa^2}\Big]\cos(qr)\Big\}. \tag{F51}$$

From Eqs. (F39) and (F50) one observes that $\mathcal{A}'^{\mathrm{h}}(0)$ as calculated in terms of $\mathscr{J}_\kappa(r)$ in Eq. (F51) (see Eq. (F37) above) has a finite limit for $\kappa\downarrow 0$, as in this limit the logarithmically divergent contributions to $\mathcal{A}'^{\mathrm{h}}(0)$ identically cancel. This cancellation can be explicitly effected through introducing the transformation $k_F r \rightharpoonup 1/[k_F r]$ in the r integral on the RHS of Eq. (F37) as applied to one of the two functions of r on the RHS of Eq. (F51). Following this, we shall be able to set κ equal to zero *prior* to evaluating the resulting total r integral.

To proceed, we note that in d spatial dimensions, $\bar{\rho}^{\mathrm{h}}(q)$ has the dimension m^{-d} (here, $d=3$), that is inverse meter to the power d. Consequently, $[\bar{\rho}^{\mathrm{h}}(q)-\bar{\rho}^{\mathrm{h}}(0)]/q$ has the dimension m^{1-d} so that $k_F^{1-d}[\bar{\rho}^{\mathrm{h}}(q)-\bar{\rho}^{\mathrm{h}}(0)]/q$ is dimensionless. Since the problem at hand has only one length scale, namely $1/k_F$, it follows that

$$\frac{[\bar{\rho}^{\mathrm{h}}(q)-\bar{\rho}^{\mathrm{h}}(0)]}{q} = k_F^{d-1}\,\mathsf{f}(q/k_F), \tag{F52}$$

where $\mathsf{f}(x)$ stands for a dimensionless function of the dimensionless variable x that has *no* explicit dependence on k_F. Consider

$$\mathsf{f}(x) \equiv \begin{cases} \mathsf{f}^<(x), & x\le 2,\\ \mathsf{f}^>(x), & x\ge 2, \end{cases} \tag{F53}$$

where we have explicitly assumed that $\mathsf{f}(x)$ is continuous at $x=2$. For $d=3$ and within the framework of the SSDA (whence the subscript ‘s’ below) we have (see Eq. (F28) above)

$$\mathsf{f}_{\mathrm{s}}^<(x) \equiv \frac{-1}{4\pi^2} + \frac{x^2}{48\pi^2}, \qquad \mathsf{f}_{\mathrm{s}}^>(x) \equiv \frac{-1}{3\pi^2 x}. \tag{F54}$$

It is seen that indeed $\mathsf{f}_{\mathrm{s}}^<(2)=\mathsf{f}_{\mathrm{s}}^>(2)$; as a matter of fact, we have also $\mathrm{d}\mathsf{f}_{\mathrm{s}}^<(x)/\mathrm{d}x\vert_{x=2} = \mathrm{d}\mathsf{f}_{\mathrm{s}}^>(x)/\mathrm{d}x\vert_{x=2}$; however, $\mathrm{d}^m\mathsf{f}_{\mathrm{s}}^<(x)/\mathrm{d}x^m\vert_{x=2} \neq \mathrm{d}^m\mathsf{f}_{\mathrm{s}}^>(x)/\mathrm{d}x^m\vert_{x=2}$ for $m\ge 2$. From Eqs. (F52) and (F53) we deduce

$$\bar{\rho}^{\mathrm{h}\prime}(0) = \lim_{q\downarrow 0}\frac{\bar{\rho}^{\mathrm{h}}(q)-\bar{\rho}^{\mathrm{h}}(0)}{q} = k_F^{d-1}\,\mathsf{f}(0) \equiv k_F^{d-1}\,\mathsf{f}^<(0). \tag{F55}$$

Further, from Eq. (F52) we have

$$\frac{\mathrm{d}}{\mathrm{d}q}\,\frac{\bar{\rho}^{\mathrm{h}}(q)-\bar{\rho}^{\mathrm{h}}(0)}{q} \equiv k_F^{d-2}\,\mathsf{f}'(q/k_F), \tag{F56}$$

where $\mathsf{f}'(x)\equiv \mathrm{d}\mathsf{f}(x)/\mathrm{d}x$.

From the expressions in Eqs. (F52) and (F56), making use of the expression in Eq. (F51), we obtain

$$\int_0^\infty \mathrm{d}r\; \mathrm{e}^{-\kappa r}\, \mathscr{J}_0(r) = \frac{k_F^2}{2}\int_0^\infty \mathrm{d}y\; \mathrm{e}^{-(\kappa/k_F)y} \times\Big\{\frac{1}{y}\int_0^\infty \mathrm{d}x\; \mathsf{f}(x/y)\sin(x) + \frac{1}{y^2}\int_0^\infty \mathrm{d}x\; \mathsf{f}'(x/y)\cos(x)\Big\}. \tag{F57}$$

In view of the result in Eq. (F39) and with reference to our above considerations, we apply the transformation $y\rightharpoonup 1/y$ in the y integral corresponding to the first term enclosed by the curly brackets on the RHS of Eq. (F57), upon which we can identify κ on the RHS of Eq. (F57) with zero; thus

$$\int_0^\infty \mathrm{d}r\; \mathrm{e}^{-\kappa r}\, \mathscr{J}_0(r) = \frac{k_F^2}{2}\int_0^\infty \frac{\mathrm{d}y}{y} \times\int_0^\infty \mathrm{d}x\; \Big\{\mathsf{f}(xy)\sin(x) + \big[\frac{\mathrm{d}}{\mathrm{d}x}\mathsf{f}(x/y)\big]\cos(x)\Big\} \equiv -\frac{k_F^2}{2}\int_0^\infty \frac{\mathrm{d}y}{y}\Big\{\mathsf{f}(0) - \int_0^\infty \mathrm{d}x\; \big[\mathsf{f}(xy)+\mathsf{f}(x/y)\big]\sin(x)\Big\}, \tag{F58}$$

where in arriving at the last expression we have assumed $\mathsf{f}(x)$ to be continuous for $x>0$ (specifically at $x=2$; see text following Eq. (F53) above) and applied integration by parts. From the result in Eq. (F58) and the defining expression for $\mathcal{A}'^{\mathrm{h}}(0)$ in Eq. (F37) above we obtain

$$\mathcal{A}'^{\mathrm{h}}(0) = \frac{2\mathsf{a}}{\pi} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 k_F^2, \tag{F59}$$

where

$$\mathsf{a} := \frac{4}{\pi} \int_0^1 \mathrm{d}y\, \mathsf{Y}(y), \tag{F60}$$

in which

$$\begin{aligned} \mathsf{Y}(y) &:= \frac{\pi^2}{y} \Big\{ \mathsf{f}(0) - \int_0^\infty \mathrm{d}x\, \big[\mathsf{f}(xy) + \mathsf{f}(x/y)\big] \sin(x) \Big\} \\ &\equiv \frac{-\pi^2}{y} \Big\{ \int_0^{2/y} \mathrm{d}x\, \big[\mathsf{f}^<(xy) - \mathsf{f}^<(0)\big] \sin(x) \\ &\quad + \int_{2/y}^\infty \mathrm{d}x\, \mathsf{f}^>(xy) \sin(x) + \int_0^{2y} \mathrm{d}x\, \mathsf{f}^<(x/y) \sin(x) \\ &\quad + \int_{2y}^\infty \mathrm{d}x\, \mathsf{f}^>(x/y) \sin(x) - \mathsf{f}^<(0) \cos(2/y) \Big\}, \end{aligned} \tag{F61}$$

where we have employed the identity

$$1 = \cos(2/y) + \int_0^{2/y} \mathrm{d}x\, \sin(x).$$

In arriving at the result in Eq. (F60) we have made use of the property

$$\mathsf{Y}(1/y) = y^2\, \mathsf{Y}(y), \tag{F62}$$

which is manifest from the first expression on the RHS of Eq. (F61), and consequently employed $\int_0^\infty \mathrm{d}y\, \mathsf{Y}(y) = 2\int_0^1 \mathrm{d}y\, \mathsf{Y}(y)$. In the light of Eqs. (F59) and (F60) and our above considerations, $\mathcal{A}'^{\mathrm{h}}(0)$ is finite provided $\mathsf{Y}(y) \sim o(1/y)$ for $y \downarrow 0$. Making use of the result in Eq. (F54), for $\mathsf{Y}(y)$ within the framework of the SSDA we obtain ($d = 3$)

$$\begin{aligned} \mathsf{Y}_{\mathrm{s}}(y) &= \frac{1 - \cos(2/y)}{4y} \\ &+ \frac{1}{24}\Big(y - (y - 2/y)\cos(2/y) - 2\sin(2/y)\Big) \\ &+ \frac{\pi/2 - \mathrm{Si}(2/y)}{3y^2} + \frac{1 - \cos(2y) - 2y\sin(2y)}{24y^3} \\ &+ \frac{1}{3}\Big(\frac{\pi}{2} - \mathrm{Si}(2y) - \frac{\cos(2y)}{2y}\Big), \end{aligned} \tag{F63}$$

where $\mathrm{Si}(z)$ stands for the sine-integral function (Abramowitz and Stegun 1972, pp. 231 and 232). From the expression in Eq. (F63) we readily deduce that

$$\mathsf{Y}_{\mathrm{s}}(y) \sim \frac{\pi}{6} - \frac{5 + 3\cos(2/y)}{24}\, y, \quad \text{for} \quad y \to 0. \tag{F64}$$

It follows that a_{s} (the value of a according to the SSDA) is indeed bounded. By means of numerical integration, we have obtained

$$\mathsf{a}_{\mathrm{s}} = 0.563\ 523\ 995\ \ldots, \tag{F65}$$

which is very close to the contribution of the RHS of Eq. (F64) to a_{s}, for which we have

$$\frac{4}{\pi} \int_0^1 \mathrm{d}y\, \Big(\frac{\pi}{6} - \frac{5 + 3\cos(2/y)}{24}\, y\Big) = 0.577\ 233\ 661\ \ldots.$$

For $\mathcal{A}_{\mathrm{s}}'^{\mathrm{h}}(0)$ we therefore have [130] (*cf.* Eq. (F59))

$$\mathcal{A}_{\mathrm{s}}'^{\mathrm{h}}(0) = \frac{2\mathsf{a}_{\mathrm{s}}}{\pi} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 k_F^2. \tag{F66}$$

With reference to our considerations in § III.E, we point out that (see footnote 83) [131]

$$\bar{\bar{\mathcal{A}}}_{\mathrm{s}}'^{\mathrm{h}}(0) \equiv \frac{\bar{\mathcal{A}}_{\mathrm{s}}'^{\mathrm{h}}(0)}{e_0^2} = \frac{2\mathsf{a}_{\mathrm{s}}}{\pi} \left(\frac{9\pi}{4}\right)^{2/3} r_s^2, \tag{F67}$$

so that in view of Eq. (108), $(2\mathsf{a}_{\mathrm{s}}/\pi)(9\pi/4)^{2/3}$ on the RHS of Eq. (F67) amounts to a contribution to $\mathcal{S}^{(2)}_{\sigma;\infty_1}(\bar{k})|_{\mathrm{s}}$. It is interesting to compare the RHS of Eq. (F67) with that of Eq. (130), taking into account that for small values of $\bar{k}/\bar{k}_F$, $\mathsf{F}(\bar{k}/\bar{k}_F) \approx 1$.

Above we have encountered $\bar{\rho}^{\mathrm{h}\prime}(0) \equiv \mathrm{d}\bar{\rho}^{\mathrm{h}}(q)/\mathrm{q}|_{q\downarrow 0}$ for a number of times. Here we consider this quantity in some detail. Note that an unbounded $\bar{\rho}^{\mathrm{h}\prime}(0) \equiv k_F^{1-d}\mathsf{f}(0)$ (see Eq. (F55) above) has through Eq. (187) a far-reaching consequence for the behaviour of the SE operator and therefore the stability of the *normal* GS assumed here (see footnote 129). Through the variable transformation $qr \rightharpoonup r$, for $q \neq 0$, in the integral on the RHS of Eq. (F44), we obtain

$$\bar{\rho}^{\mathrm{h}\prime}(0) = \lim_{q\downarrow 0} \frac{4\pi}{q^4} \int_0^\infty \mathrm{d}r\, r^2\, \rho^{\mathrm{h}}(r/q) \Big[\cos(r) - \frac{\sin(r)}{r}\Big]. \tag{F68}$$

From this expression it is seen that for $\bar{\rho}^{\mathrm{h}\prime}(0)$ to be bounded, it is required that for $q \downarrow 0$ the integral on the RHS approach zero like q^α, with $\alpha \geq 4$: $\alpha = 4$ gives rise to a finite $\bar{\rho}^{\mathrm{h}\prime}(0)$, whereas $\alpha > 4$ yields a vanishing $\bar{\rho}^{\mathrm{h}\prime}(0)$; the possibility of $\alpha < 4$ corresponds to an unbounded $\bar{\rho}^{\mathrm{h}\prime}(0)$ which contradicts the result in Eq. (F43). Since for any *finite* value of q, the integrand of the r integral on the RHS of Eq. (F68) behaves like r^4 for $(r/q) \downarrow 0$, the *leading* term in the AS of this integral for $q \downarrow 0$ is determined by the behaviour of $\rho^{\mathrm{h}}(r)$ for $r \to \infty$. This implies

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[130] The author should like to thank Professor Roland Zimmermann whose expression of concern with regard to the possibility of unboundedness of $\mathcal{A}_{\mathrm{s}}'^{\mathrm{h}}(0)$ led the author to detect an error in the original derivation of the result in Eq. (F66), causing a_{s} herein to be incorrectly identified with unity; the same error had caused the constant a on the RHS of Eq. (F59) to be different from that in Eq. (F60) above.

[131] $(2\mathsf{a}_{\mathrm{s}}/\pi)\,(9\pi/4)^{2/3} \approx 2.34\,\mathsf{a}_{\mathrm{s}} \approx 1.32$.

that $\bar{\rho}^{\rm h\prime}(0)$ is fully determined by the leading term in the large-r AS of $\rho^{\rm h}(r)$. It is here that the knowledge of this term proves most useful. Within the SSDA, making use of Eq. (F19) we have

$$\rho_{\rm s}^{\rm h}(r/q) \equiv \sum_{\sigma'} \big(\varrho_{{\rm s};\sigma'}^{\rm h}(r/q)\big)^2 \sim \frac{k_F^2}{2\pi^4}\, q^4\, \frac{\cos^2(k_F\, r/q)}{r^4}, \tag{F69}$$

from which and Eq. (F68), making use of the standard integral

$$\int_0^\infty {\rm d}r\, \frac{\cos^2(\alpha r)}{r^2} \Big[\cos(r) - \frac{\sin(r)}{r}\Big] = -\frac{\pi}{8}, \quad \alpha \neq 0, \tag{F70}$$

we obtain

$$\bar{\rho}_{\rm s}^{\rm h\prime}(0) = -\frac{k_F^2}{4\pi^2}, \tag{F71}$$

which is exactly the result obtained from Eqs. (F54) and (F56) above for $d = 3$.

Below, in § F.1.c, we consider the behaviour of the *exact* $\rho^{\rm h}(r)$ in some detail. Here we deduce an approximate expression for this function in the regime of weak interaction. From our above considerations, making use of Eq. (F55) above and the approximate expression in Eq. (F101) below, we obtain

$$\mathsf{f}(0) \approx \Big[Z_F^2 + |C_{\bf 0}|^2 (1 - Z_F)^2\Big]\, \mathsf{f}_{\rm s}(0), \tag{F72}$$

where $C_{\bf 0}$ denotes the overlap of the *exact* N-particle GS of the system with the N-particle GS of the non-interacting system (see Eq. (F81) below). From Eq. (F54) above we have $\mathsf{f}_{\rm s}(0) = -1/[4\pi^2]$.

Since in practice one calculates $\Gamma^{(m)}$, $m = 1, 2, \dots$, rather than, say, $\mathcal{U}(\boldsymbol{r}_1'', \boldsymbol{r}_2'')$ as defined in Eq. (F4), the expression for $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ in Eq. (F3) is not useful. To obtain a practically useful expression, we make use of Eq. (F2) which in fact *defines* $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$. Through some rearrangement of terms, we obtain the following result

$$\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}') = \int {\rm d}^d r_1''\; v(\boldsymbol{r} - \boldsymbol{r}_1'') \Big\{ v(\boldsymbol{r}' - \boldsymbol{r}_1'') n(\boldsymbol{r}_1'') + \int {\rm d}^d r_2''\; v(\boldsymbol{r}' - \boldsymbol{r}_2'') \sum_{\sigma_1', \sigma_2'} \Big[\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'; \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2') - n_{\sigma_1'}(\boldsymbol{r}_1'') n_{\sigma_2'}(\boldsymbol{r}_2'') \Big] \Big\}. \tag{F73}$$

We emphasize that in evaluating the $\boldsymbol{r}_1''$ integral it is important (it is even vital, when $v \equiv v_c$) not to separate the terms enclosed by the curly brackets, since cancellation among these terms plays a crucial role in rendering the integrand sufficiently rapidly decaying for large values of $\|\boldsymbol{r}_1''\|$.

Finally, from Eq. (F73) for $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ within the framework of the SSDA (see Appendix C) we obtain

$$\mathcal{A}_{\rm s}'(\boldsymbol{r}, \boldsymbol{r}') = \int {\rm d}^d r_1''\; v(\boldsymbol{r} - \boldsymbol{r}_1'') \Big\{ v(\boldsymbol{r}' - \boldsymbol{r}_1'') n(\boldsymbol{r}_1'') - \int {\rm d}^d r_2''\; v(\boldsymbol{r}' - \boldsymbol{r}_2'') \sum_{\sigma'} \varrho_{{\rm s};\sigma'}^2(\boldsymbol{r}_1'', \boldsymbol{r}_2'') \Big\}. \tag{F74}$$

We have already dealt with this expression (see Eqs. (F16) and (F18) above) while considering uniform and isotropic GSs.

c. On the behaviour of $\rho(\boldsymbol{r}, \boldsymbol{r}')$ pertaining to uniform and isotropic ground states

In § 1 of this Appendix, we introduced the function $\rho(\boldsymbol{r}_1'', \boldsymbol{r}_2'')$ (see Eq. (F13)) which according to the SSDA is equal to $\sum_{\sigma'} \varrho_{{\rm s};\sigma'}^2(\boldsymbol{r}_1'', \boldsymbol{r}_2'')$. Here we analyse $\rho(\boldsymbol{r}_1'', \boldsymbol{r}_2'')$ pertaining to uniform GSs is some detail and deduce the behaviour of the leading-order term in the AS of this function for $\|\boldsymbol{r}_1'' - \boldsymbol{r}_2''\| \to \infty$.

Making use of Eq. (A41), from Eq. (B1) we obtain

$$\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'; \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2') = \frac{-1}{\Omega^2} \sum_{\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{k}_3} \times \langle \Psi_{N;0} | \hat{\mathsf{a}}_{\boldsymbol{k}_1;\sigma_1'}^\dagger \hat{\mathsf{a}}_{\boldsymbol{k}_2;\sigma_2'}^\dagger \hat{\mathsf{a}}_{\boldsymbol{k}_3;\sigma_1'} \hat{\mathsf{a}}_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3;\sigma_2'} | \Psi_{N;0} \rangle \times {\rm e}^{-i(\boldsymbol{k}_1 - \boldsymbol{k}_3)\cdot(\boldsymbol{r}_1'' - \boldsymbol{r}_2'')}, \tag{F75}$$

where we have made use of

$$\langle \Psi_{N;0} | \hat{\mathsf{a}}_{\boldsymbol{k}_1;\sigma_1'}^\dagger \hat{\mathsf{a}}_{\boldsymbol{k}_2;\sigma_2'}^\dagger \hat{\mathsf{a}}_{\boldsymbol{k}_3;\sigma_1'} \hat{\mathsf{a}}_{\boldsymbol{k}_4;\sigma_2'} | \Psi_{N;0} \rangle \propto \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2, \boldsymbol{k}_3+\boldsymbol{k}_4}. \tag{F76}$$

Let now $\{|\boldsymbol{\xi}\rangle\}$ be the complete set of normalized N-particle Slater determinants, composed of single-particle states $\{|\boldsymbol{k}\rangle\}$, $\langle \boldsymbol{r}|\boldsymbol{k}\rangle = \Omega^{-1/2} \exp(i\boldsymbol{k}\cdot\boldsymbol{r})$, corresponding to the *same* set $\{N_\sigma\}$ of partial number-operators eigenvalues as that corresponding to the interacting GS $|\Psi_{N;0}\rangle$. We identify $\boldsymbol{\xi}$ with a vector of N components, comprised of $2\mathsf{s}+1$ sub-vectors $\boldsymbol{\xi}_i$ of N_{σ_i} components, where $i = 1, \dots, 2\mathsf{s}+1$. That is

$$\boldsymbol{\xi} \equiv \boldsymbol{\xi}_{\sigma_1}, \dots, \boldsymbol{\xi}_{\sigma_{2\mathsf{s}+1}}. \tag{F77}$$

For $N_{\sigma_i} \neq 0$, each component of $\boldsymbol{\xi}_{\sigma_i}$ is equal to a non-vanishing wave-vector $\boldsymbol{k}$ and, by antisymmetry, *no* two vectors (provided that $N_{\sigma_i} \geq 2$) in $\boldsymbol{\xi}_{\sigma_i}$ are identical. Further, by the *indistinguishability* of the particles, any vector $\tilde{\boldsymbol{\xi}}_{\sigma_i}$ whose wave-vector components are by permutation related to those of $\boldsymbol{\xi}_{\sigma_i}$ are identified as representing the *same* vector, that is $\boldsymbol{\xi}_{\sigma_i}$. [132] Below, we denote the $\boldsymbol{\xi}$

[132] When *all* N_{σ_i} except one are vanishing, $|\boldsymbol{\xi}\rangle$ describes a fully spin-polarized state.

associated with the Slater determinant of lowest (kinetic) energy by $\boldsymbol{\xi} = \mathbf{0}$ so that (see Appendix C)

$$|\mathbf{0}\rangle := |\boldsymbol{\xi} = \mathbf{0}\rangle \equiv |\Phi_{N;0}\rangle; \tag{F78}$$

the symbol $|\mathbf{0}\rangle$ should not be confused with the single-particle state $|\boldsymbol{k}\rangle$ for $\boldsymbol{k} = \mathbf{0}$.

Expanding $|\Psi_{N;0}\rangle$ with respect to the complete set $\{|\boldsymbol{\xi}\rangle\}$, we have

$$|\Psi_{N;0}\rangle = \sum_{\boldsymbol{\xi}} C_{\boldsymbol{\xi}}\, |\boldsymbol{\xi}\rangle \equiv \sum_{\boldsymbol{\xi}_{\sigma_1},\dots,\boldsymbol{\xi}_{\sigma_{2s+1}}} C_{\boldsymbol{\xi}_{\sigma_1},\dots,\boldsymbol{\xi}_{\sigma_{2s+1}}}\, |\boldsymbol{\xi}_{\sigma_1},\dots,\boldsymbol{\xi}_{\sigma_{2s+1}}\rangle; \tag{F79}$$

completeness of $\{|\boldsymbol{\xi}\rangle\}$ together with the normalization to unity of both $|\Psi_{N;0}\rangle$ and $\{|\boldsymbol{\xi}\rangle\}$ imply that

$$\sum_{\boldsymbol{\xi}} |C_{\boldsymbol{\xi}}|^2 \equiv \sum_{\boldsymbol{\xi}_{\sigma_1},\dots,\boldsymbol{\xi}_{\sigma_{2s+1}}} |C_{\boldsymbol{\xi}_{\sigma_1},\dots,\boldsymbol{\xi}_{\sigma_{2s+1}}}|^2 = 1 \tag{F80}$$

and

$$C_{\boldsymbol{\xi}} = \langle \boldsymbol{\xi} | \Psi_{N;0}\rangle. \tag{F81}$$

Following the above considerations, we can now write

$$\begin{aligned}
&\langle\Psi_{N;0}|\hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_1;\sigma_1'} \hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_2;\sigma_2'} \hat{\mathsf{a}}_{\boldsymbol{k}_3;\sigma_1'} \hat{\mathsf{a}}_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3;\sigma_2'}|\Psi_{N;0}\rangle \\
&\quad = \sum_{\boldsymbol{\xi}} |C_{\boldsymbol{\xi}}|^2\, \langle\boldsymbol{\xi}|\hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_1;\sigma_1'} \hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_2;\sigma_2'} \hat{\mathsf{a}}_{\boldsymbol{k}_3;\sigma_1'} \hat{\mathsf{a}}_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3;\sigma_2'}|\boldsymbol{\xi}\rangle \\
&\quad +\delta\langle\Psi_{N;0}|\hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_1;\sigma_1'} \hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_2;\sigma_2'} \hat{\mathsf{a}}_{\boldsymbol{k}_3;\sigma_1'} \hat{\mathsf{a}}_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3;\sigma_2'}|\Psi_{N;0}\rangle,
\end{aligned} \tag{F82}$$

where

$$\begin{aligned}
&\delta\langle\Psi_{N;0}|\hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_1;\sigma_1'} \hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_2;\sigma_2'} \hat{\mathsf{a}}_{\boldsymbol{k}_3;\sigma_1'} \hat{\mathsf{a}}_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3;\sigma_2'}|\Psi_{N;0}\rangle \\
&:= \sum_{\substack{\boldsymbol{\xi},\boldsymbol{\xi}' \\ (\boldsymbol{\xi}\neq\boldsymbol{\xi}')}} C^*_{\boldsymbol{\xi}}\, C_{\boldsymbol{\xi}'}\, \langle\boldsymbol{\xi}|\hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_1;\sigma_1'} \hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_2;\sigma_2'} \hat{\mathsf{a}}_{\boldsymbol{k}_3;\sigma_1'} \hat{\mathsf{a}}_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3;\sigma_2'}|\boldsymbol{\xi}'\rangle.
\end{aligned} \tag{F83}$$

For the reason that will become evident shortly, it is advantageous to express the matrix element in the first term on the RHS of Eq. (F82) in terms of the coordinate representation of $\Gamma^{(2)}_{\boldsymbol{\xi}}$ defined in Eq. (C4); making use of the expression in Eq. (A40), one readily verifies that

$$\begin{aligned}
&\langle\boldsymbol{\xi}|\hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_1;\sigma_1'} \hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k}_2;\sigma_2'} \hat{\mathsf{a}}_{\boldsymbol{k}_3;\sigma_1'} \hat{\mathsf{a}}_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3;\sigma_2'}|\boldsymbol{\xi}\rangle \\
&\quad = \frac{-1}{\Omega^2} \int \Pi_{j=1}^4 \mathrm{d}^d r_j\, \Gamma^{(2)}_{\boldsymbol{\xi}}(\boldsymbol{r}_1\sigma_1', \boldsymbol{r}_2\sigma_2'; \boldsymbol{r}_3\sigma_1', \boldsymbol{r}_4\sigma_2') \\
&\qquad \times \mathrm{e}^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_1}\, \mathrm{e}^{i\boldsymbol{k}_2\cdot\boldsymbol{r}_2}\, \mathrm{e}^{-i\boldsymbol{k}_3\cdot\boldsymbol{r}_3}\, \mathrm{e}^{-i(\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3)\cdot\boldsymbol{r}_4}.
\end{aligned} \tag{F84}$$

Since $|\boldsymbol{\xi}\rangle$ is a single Slater determinant, for $\boldsymbol{\xi} = \mathbf{0}$, $\Gamma^{(2)}_{\boldsymbol{\xi}}$ exactly coincides with $\Gamma^{(2)}_{\mathrm{s}}$ which we have defined in Appendix C. Denoting the generalized Slater-Fock density matrix corresponding to $|\boldsymbol{\xi}\rangle$, by $\varrho_{\boldsymbol{\xi};\sigma}(\boldsymbol{r},\boldsymbol{r}')$, defined according to (*cf.* Eq. (F24) above)

$$\begin{aligned}
\varrho_{\boldsymbol{\xi};\sigma}(\boldsymbol{r},\boldsymbol{r}') &:= \langle\boldsymbol{\xi}|\hat{\psi}^{\dagger}_{\sigma}(\boldsymbol{r})\hat{\psi}_{\sigma}(\boldsymbol{r}')|\boldsymbol{\xi}\rangle \\
&= \frac{1}{\Omega} \sum_{\boldsymbol{k}\in\boldsymbol{\xi}_{\sigma}} \exp(-i\boldsymbol{k}\cdot[\boldsymbol{r}-\boldsymbol{r}']),
\end{aligned} \tag{F85}$$

where by $\boldsymbol{k} \in \boldsymbol{\xi}_{\sigma}$ we specify that $\boldsymbol{k}$ is one of the N_{σ} *non-vanishing* components of vector $\boldsymbol{\xi}_{\sigma}$, we have (see Appendix C, the paragraph following that containing Eq. (C4))

$$\begin{aligned}
\Gamma^{(2)}_{\boldsymbol{\xi}}(\boldsymbol{r}_1\sigma_1', \boldsymbol{r}_2\sigma_2'; \boldsymbol{r}_3\sigma_1', \boldsymbol{r}_4\sigma_2') &= \varrho_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r}_1,\boldsymbol{r}_3)\, \varrho_{\boldsymbol{\xi};\sigma_2'}(\boldsymbol{r}_2,\boldsymbol{r}_4) \\
&\quad -\delta_{\sigma_1',\sigma_2'}\, \varrho_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r}_1,\boldsymbol{r}_4)\, \varrho_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r}_2,\boldsymbol{r}_3).
\end{aligned} \tag{F86}$$

This simplified result clarifies our use of the representation in Eq. (F84). We point out that, similar to $\varrho_{\mathrm{s};\sigma}$, $\varrho_{\boldsymbol{\xi};\sigma}$ is *idempotent*, that is (*cf.* Eq. (166))

$$\int \mathrm{d}^d r''\; \varrho_{\boldsymbol{\xi};\sigma}(\boldsymbol{r},\boldsymbol{r}'')\varrho_{\boldsymbol{\xi};\sigma}(\boldsymbol{r}'',\boldsymbol{r}') = \varrho_{\boldsymbol{\xi};\sigma}(\boldsymbol{r},\boldsymbol{r}'). \tag{F87}$$

The validity of this expression is readily verified through employing the second expression on the RHS of Eq. (F85) for $\varrho_{\boldsymbol{\xi};\sigma}$ on both sides of Eq. (F87).

Substituting the RHS of Eq. (F86) into that of Eq. (F84), from Eqs. (F75) and (F82), upon exchange of orders of wave-vector summations and spatial integrations, we obtain

$$\begin{aligned}
\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'; \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2') &= -\delta_{\sigma_1',\sigma_2'} \sum_{\boldsymbol{\xi}} |C_{\boldsymbol{\xi}}|^2 \\
&\quad \times \varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r}_1''-\boldsymbol{r}_2'')\, \varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma_1'}(-\boldsymbol{r}_1''+\boldsymbol{r}_2'') \\
&\quad + \sum_{\boldsymbol{\xi}} |C_{\boldsymbol{\xi}}|^2\, \varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi},\sigma_1'}(\mathbf{0})\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi},\sigma_2'}(\mathbf{0}) \\
&\quad +\delta\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'; \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'),
\end{aligned} \tag{F88}$$

where we have introduced (*cf.* Eq. (F9))

$$\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma}(\boldsymbol{r}-\boldsymbol{r}') \equiv \varrho_{\boldsymbol{\xi};\sigma}(\boldsymbol{r},\boldsymbol{r}') \tag{F89}$$

and where $\delta\Gamma^{(2)}$ is the contribution due to the second term on the RHS of Eq. (F82). We note that, with the exception of the case where $\boldsymbol{\xi} = \mathbf{0}$, $\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma}(\boldsymbol{r})$ is *not* isotropic. This we have signified by means of the superscript '¬i'; thus although the function in question is invariant under a simultaneous continuous translation of $\boldsymbol{r}$ and $\boldsymbol{r}'$ (it is 'homogeneous', as signified by the superscript 'h'), it is *not* necessarily a function of

$\|\boldsymbol{r}-\boldsymbol{r}'\|$ (i.e. not necessarily 'isotropic'). It can, however, be shown that by time-reversal symmetry, $|C_{\boldsymbol{\xi}}|^2 = |C_{-\boldsymbol{\xi}}|^2$, where $-\boldsymbol{\xi}$, the 'time-reversed' counterpart of $\boldsymbol{\xi}$, denotes the vector obtained from $\boldsymbol{\xi}$ through multiplying *all* component wave-vectors herein by -1. Consequently, the RHS of Eq. (F88) is indeed an isotropic function of $\boldsymbol{r}_1''-\boldsymbol{r}_2''$. For completeness, we mention that, in arriving at the expression in Eq. (F88), we have replaced $\varrho_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r}_1,\boldsymbol{r}_1-\boldsymbol{r}_1''+\boldsymbol{r}_2'')$, $\varrho_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r}_1-\boldsymbol{r}_1''+\boldsymbol{r}_2'',\boldsymbol{r}_1)$, $\varrho_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r}_1,\boldsymbol{r}_1)$, and $\varrho_{\boldsymbol{\xi};\sigma_2'}(\boldsymbol{r}_1-\boldsymbol{r}_1''+\boldsymbol{r}_2'',\boldsymbol{r}_1-\boldsymbol{r}_1''+\boldsymbol{r}_2'')$ by the equivalent functions $\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r}_1'-\boldsymbol{r}_2'')$, $\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma_1'}(-\boldsymbol{r}_1'+\boldsymbol{r}_2'')$, $\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{0})$ and $\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma_2'}(\boldsymbol{0})$ respectively.

In view of the fact that

$$\mathsf{n}_{\boldsymbol{\xi};\sigma}(\boldsymbol{k}) := \langle\boldsymbol{\xi}|\hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k};\sigma}\hat{\mathsf{a}}_{\boldsymbol{k};\sigma}|\boldsymbol{\xi}\rangle \tag{F90}$$

is the Fourier transform with respect to $\boldsymbol{r}$ of [133] $\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma}(\boldsymbol{r})$, by introducing

$$\delta\varrho_{\boldsymbol{\xi};\sigma}(\boldsymbol{r},\boldsymbol{r}') := \varrho_{\boldsymbol{\xi};\sigma}(\boldsymbol{r},\boldsymbol{r}') - \varrho_{\sigma}(\boldsymbol{r},\boldsymbol{r}'), \tag{F91}$$

we have the following associated expression

$$\delta\mathsf{n}_{\boldsymbol{\xi};\sigma}(\boldsymbol{k}) := \mathsf{n}_{\boldsymbol{\xi};\sigma}(\boldsymbol{k}) - \mathsf{n}_{\sigma}(k); \tag{F92}$$

note that, unless $\boldsymbol{\xi}=\boldsymbol{0}$, this function depends on both the magnitude and direction of $\boldsymbol{k}$ (see our remarks following Eq. (F89) above). Since the momentum-distribution functions $\mathsf{n}_{\boldsymbol{\xi};\sigma}(\boldsymbol{k})$, $\forall\boldsymbol{\xi}$, are defined with respect to the N-particle states corresponding to the same set of values $\{N_\sigma\}$ as corresponding to the GS of the interacting system, from Eq. (J3) (see also Eq. (H10)) we immediately deduce the useful result

$$\sum_{\boldsymbol{k}} \delta\mathsf{n}_{\boldsymbol{\xi};\sigma}(\boldsymbol{k}) = 0 \iff \delta\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma}(\boldsymbol{r}=\boldsymbol{0}) = 0. \tag{F93}$$

Further, through multiplying both sides of Eq. (F92) by $|C_{\boldsymbol{\xi}}|^2$ (note that $\langle\boldsymbol{\xi}|\hat{\mathsf{a}}^{\dagger}_{\boldsymbol{k};\sigma}\hat{\mathsf{a}}_{\boldsymbol{k};\sigma}|\boldsymbol{\xi}'\rangle \propto \delta_{\boldsymbol{\xi},\boldsymbol{\xi}'}$) and summing over all $\boldsymbol{\xi}$, from Eq. (F80) we obtain the following equally useful result:

$$\sum_{\boldsymbol{\xi}} |C_{\boldsymbol{\xi}}|^2\, \delta\mathsf{n}_{\boldsymbol{\xi};\sigma}(\boldsymbol{k}) = 0, \tag{F94}$$

which is equivalent with (*cf.* Eq. (J3))

$$\sum_{\boldsymbol{\xi}} |C_{\boldsymbol{\xi}}|^2\, \delta\varrho_{\boldsymbol{\xi};\sigma}(\boldsymbol{r},\boldsymbol{r}') \equiv 0. \tag{F95}$$

Consequently, making use of Eq. (F91) we obtain

$$\sum_{\boldsymbol{\xi}} |C_{\boldsymbol{\xi}}|^2\, \varrho_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r},\boldsymbol{r}')\,\varrho_{\boldsymbol{\xi};\sigma_2'}(\boldsymbol{r}',\boldsymbol{r}) \equiv \varrho_{\sigma_1'}(\boldsymbol{r},\boldsymbol{r}')\varrho_{\sigma_2'}(\boldsymbol{r}',\boldsymbol{r}) + \sum_{\boldsymbol{\xi}} |C_{\boldsymbol{\xi}}|^2 \delta\varrho_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r},\boldsymbol{r}')\,\delta\varrho_{\boldsymbol{\xi};\sigma_2'}(\boldsymbol{r}',\boldsymbol{r}). \tag{F96}$$

In view of the second of the results in Eq. (F93), as well as the expression in Eq. (F80), identification of $\boldsymbol{r}'$ with $\boldsymbol{r}$ in Eq. (F96) leads to an *identity*, reflecting the equality of the sets of particles concentrations, $\{n_{0;\sigma}\}$, associated with all the N-particle states involved (see the paragraph directly following Eq. (F76) above). Making use of the result in Eq. (F96), we can re-write Eq. (F88) as follows

$$\begin{aligned}\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2';\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2') &= n_{0;\sigma_1'}n_{0;\sigma_2'}\\ &-\delta_{\sigma_1',\sigma_2'}\Big(\varrho^2_{\sigma_1'}(\boldsymbol{r}_1'',\boldsymbol{r}_2'') + \sum_{\boldsymbol{\xi}} |C_{\boldsymbol{\xi}}|^2\, \delta\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r}_1''-\boldsymbol{r}_2'')\\ &\qquad\times\delta\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma_1'}(\boldsymbol{r}_2''-\boldsymbol{r}_1'')\Big)\\ &+\delta\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2';\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2').\end{aligned} \tag{F97}$$

It is interesting to note that neglecting $\delta\Gamma^{(2)}$, the off-diagonal elements of $\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2';\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2')$ in the spin space are solely determined by $\{n_{0;\sigma}\}$. Making use of the expression in Eq. (F97), from Eq. (F13) we finally obtain

$$\begin{aligned}\rho(\boldsymbol{r}_1'',\boldsymbol{r}_2'') &= \sum_{\sigma'} \varrho^2_{\sigma'}(\boldsymbol{r}_1'',\boldsymbol{r}_2'')\\ &+\sum_{\boldsymbol{\xi}} |C_{\boldsymbol{\xi}}|^2 \sum_{\sigma'} \delta\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma'}(\boldsymbol{r}_1''-\boldsymbol{r}_2'')\,\delta\varrho^{\mathrm{h}\neg\mathrm{i}}_{\boldsymbol{\xi};\sigma'}(\boldsymbol{r}_2''-\boldsymbol{r}_1'')\\ &+\delta\rho(\boldsymbol{r}_1'',\boldsymbol{r}_2''),\end{aligned} \tag{F98}$$

which is our desired result. Here $\delta\rho(\boldsymbol{r}_1'',\boldsymbol{r}_2'')$ is the contribution due to $\delta\Gamma^{(2)}$ on the RHS of Eq. (F97).

The expression in Eq. (F98) provides us with some *insight* concerning the leading asymptotic behaviour of $\rho(\boldsymbol{r}_1'',\boldsymbol{r}_2'')$, for $\|\boldsymbol{r}_1''-\boldsymbol{r}_2''\|\to\infty$, at least in the case of weakly interacting systems. In such systems, by appealing to properties (see Eq. (F80) above)

$$|C_{\boldsymbol{0}}| \approx 1 \;\;\text{and thus}\;\; |C_{\boldsymbol{\xi}}| \approx 0 \;\text{for}\; \boldsymbol{\xi}\neq\boldsymbol{0}, \tag{F99}$$

we restrict the sum over $\boldsymbol{\xi}$ on the RHS of Eq. (F98) to the term corresponding to $\boldsymbol{\xi}=\boldsymbol{0}$, which upon using Eq. (F99) results in

$$\begin{aligned}\rho(\boldsymbol{r}_1'',\boldsymbol{r}_2'') \approx \sum_{\sigma'}\Big\{&\big(1+|C_{\boldsymbol{0}}|^2\big)\big(\varrho^{\mathrm{h}}_{\sigma'}(\|\boldsymbol{r}_1''-\boldsymbol{r}_2''\|)\big)^2\\ &+|C_{\boldsymbol{0}}|^2\,\varrho^{\mathrm{h}}_{0;\sigma'}(\|\boldsymbol{r}_1''-\boldsymbol{r}_2''\|)\\ &-2|C_{\boldsymbol{0}}|^2\,\varrho^{\mathrm{h}}_{0;\sigma'}(\|\boldsymbol{r}_1''-\boldsymbol{r}_2''\|)\big(\varrho^{\mathrm{h}}_{\sigma'}(\|\boldsymbol{r}_1''-\boldsymbol{r}_2''\|)\big)^2\Big\}.\end{aligned} \tag{F100}$$

We note that $\delta\rho(\boldsymbol{r}_1'',\boldsymbol{r}_2'')$ on the RHS of Eq. (F98) has *not* been incorporated in the expression on the RHS of

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[133] This holds equally true for $\mathsf{n}_\sigma(k)$, the momentum distribution function pertaining to uniform and isotropic interacting GSs defined in Eq. (J2), which is the Fourier transform with respect to $\boldsymbol{r}$ of $\varrho^{\mathrm{h}}_{\sigma}(\|\boldsymbol{r}\|)$ (see Eq. (J3)).

Eq. (F100), following the fact that the sum on the RHS of Eq. (F83) involves $C^*_{\boldsymbol{\xi}} C_{\boldsymbol{\xi}'}$ with $\boldsymbol{\xi} \neq \boldsymbol{\xi}'$ so that *at least* one of $C_{\boldsymbol{\xi}}$ and $C_{\boldsymbol{\xi}'}$ is *not* equal to $C_{\mathbf{0}}$.

From Eq. (F100) and the result in Eq. (J6) we obtain the following *approximate* leading-order asymptotic result

$$\rho^{\mathrm{h}}(r) \sim \sum_{\sigma} \frac{k_{F;\sigma}^2}{4\pi^4} \big[Z_{F;\sigma}^2 + |C_{\mathbf{0}}|^2 (1 - Z_{F;\sigma})^2\big] \times \frac{\cos^2(k_{F;\sigma}\, r)}{r^4}, \quad r \to \infty, \tag{F101}$$

where (*cf.* Eq. (F9))

$$\rho^{\mathrm{h}}(r) \equiv \rho^{\mathrm{h}}(\|\boldsymbol{r}\|) := \rho(\boldsymbol{r}, \mathbf{0}). \tag{F102}$$

For weakly-interacting fermions, $Z_{F;\sigma}$ is close to unity, so that $|C_{\mathbf{0}}|^2 (1 - Z_{F;\sigma})^2$ in Eq. (F101) can be neglected in comparison with $Z_{F;\sigma}^2$, in which case $\rho^{\mathrm{h}}(r)$ at large r is seen not to depend *explicitly* on $C_{\mathbf{0}}$.

d. On the van Hove pair correlation function $\mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r}, \boldsymbol{r}')$

From Eqs. (B21) and (F97), for the normalized van Hove pair correlation function pertaining to a uniform and isotropic system we have

$$\begin{aligned} \mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r}, \boldsymbol{r}') = {}& \frac{n_{0;\sigma} n_{0;\sigma'}}{n_0^2} - \frac{1}{n_0^2} \Big\{ \varrho_\sigma^2(\boldsymbol{r}, \boldsymbol{r}') \\ & + \sum_{\boldsymbol{\xi}} |C_{\boldsymbol{\xi}}|^2\, \delta\varrho_{\boldsymbol{\xi};\sigma}^{\mathrm{h}\neg\mathrm{i}}(\boldsymbol{r} - \boldsymbol{r}')\, \delta\varrho_{\boldsymbol{\xi};\sigma}^{\mathrm{h}\neg\mathrm{i}}(\boldsymbol{r}' - \boldsymbol{r}) \Big\}\, \delta_{\sigma,\sigma'} \\ & + \delta\mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r}, \boldsymbol{r}'), \end{aligned} \tag{F103}$$

where $\delta\mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r}, \boldsymbol{r}')$ denotes the contribution associated with $\delta\Gamma^{(2)}$ on the RHS of Eq. (F97). With (see Eq. (F9) above)

$$\mathsf{g}_{\sigma,\sigma'}^{\mathrm{h}}(r) \equiv \mathsf{g}_{\sigma,\sigma'}^{\mathrm{h}}(\|\boldsymbol{r}\|) := \mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r}, \mathbf{0}), \tag{F104}$$

under the assumption of the validity of the assertions in Eq. (F99), from Eq. (F103) we readily obtain

$$\mathsf{g}_{\sigma,\sigma'}^{\mathrm{h}}(r) \sim \frac{n_{0;\sigma} n_{0;\sigma'}}{n_0^2} - \frac{k_{F;\sigma}^2 \big[Z_{F;\sigma}^2 + |C_{\mathbf{0}}|^2 (1 - Z_{F;\sigma})^2\big]}{4\pi^4\, n_0^2} \times \frac{\cos^2(k_{F;\sigma}\, r)}{r^4}\, \delta_{\sigma,\sigma'}, \quad r \to \infty, \tag{F105}$$

where we have made use of the asymptotic results in Eqs. (F19) and (J6). In practice one often deals with the following function

$$\mathsf{g}^{\mathrm{h}}(r) := \sum_{\sigma,\sigma'} \mathsf{g}_{\sigma,\sigma'}^{\mathrm{h}}(r), \tag{F106}$$

for which from Eq. (F105) one readily obtains the following result

$$\mathsf{g}^{\mathrm{h}}(r) \sim 1 - \frac{1}{n_0^2} \sum_{\sigma} \frac{k_{F;\sigma}^2}{4\pi^4} \big[Z_{F;\sigma}^2 + |C_{\mathbf{0}}|^2 (1 - Z_{F;\sigma})^2\big] \times \frac{\cos^2(k_{F;\sigma}\, r)}{r^4}, \quad r \to \infty. \tag{F107}$$

Note that the second term on the RHS of Eq. (F107) is equal to $1/n_0^2$ times the RHS of Eq. (F101). For uniform system of spin-1/2 fermions in the paramagnetic phase, where $k_{F;\sigma} = k_F$ and $Z_{F;\sigma} = Z_F$, Eq. (F107) takes on the following simple form

$$\mathsf{g}^{\mathrm{h}}(r) \sim 1 - \frac{9\big[Z_F^2 + |C_{\mathbf{0}}|^2 (1 - Z_F)^2\big]}{2k_F^4}\, \frac{\cos^2(k_F\, r)}{r^4}, \; r \to \infty. \tag{F108}$$

The result in Eq. (F108) is interesting in that it exposes that at least for weakly interacting systems, for which the conditions in Eq. (F99) apply, $\rho^{\mathrm{h}}(r) \sim n_0^2\big(1 - \mathsf{g}^{\mathrm{h}}(r)\big)$ for large values of r. Note in passing that the appropriate expressions for $\mathsf{g}_{\sigma,\sigma'}^{\mathrm{h}}(r)$ and $\mathsf{g}^{\mathrm{h}}(r)$ within the framework of the SSDA are readily obtained through identifying with unity both $|C_{\mathbf{0}}|^2$ and $Z_{F;\sigma}$ in Eqs. (F105) and (F107). It is important to realize that, although the approximate result in for instance Eq. (F108) relies on the conditions in Eq. (F99), nonetheless it is far superior to the straightforward approximation in which the series on the RHS of Eq. (F79) is restricted to its first term, namely $C_{\mathbf{0}}|\mathbf{0}\rangle$; such an approximation would have resulted in $|C_{\mathbf{0}}|^2$ as being the first term on RHS of Eq. (F107), rather than the present *exact* result 1. Although this may not seem an important aspect in the first glance, the fact that $|C_{\mathbf{0}}|^2 \neq 1$ (unless the system under consideration is fully non-interacting), $\mathsf{g}^{\mathrm{h}}(r) \sim |C_{\mathbf{0}}|^2$ for $r \to \infty$ amounts to a fundamental error as regards the charge conservation in the system.

2. $\mathcal{B}_\sigma(\boldsymbol{r}, \boldsymbol{r}')$ and its regularized forms $\mathcal{B}'_\sigma(\boldsymbol{r}, \boldsymbol{r}')$ and $\mathcal{B}''_\sigma(\boldsymbol{r}, \boldsymbol{r}')$

Here we deal with $\mathcal{B}_\sigma(\boldsymbol{r}, \boldsymbol{r}')$; however, contrary to the case of $\mathcal{A}(\boldsymbol{r}, \boldsymbol{r}')$ we shall not go into the details which are very similar to those underlying regularization of $\mathcal{A}(\boldsymbol{r}, \boldsymbol{r}')$.

Making use of the anticommutation relations in Eq. (29) and the defining expression for $\Gamma^{(2)}$ in Eq. (B1), we obtain

$$\begin{aligned} \Gamma^{(2)}(\boldsymbol{r}'\sigma, \boldsymbol{r}''\sigma'; \boldsymbol{r}''\sigma', \boldsymbol{r}\sigma) = {}& \delta_{\sigma,\sigma'}\delta(\boldsymbol{r}' - \boldsymbol{r}'')\, \varrho_\sigma(\boldsymbol{r}', \boldsymbol{r}) \\ & - n_{\sigma'}(\boldsymbol{r}'') \varrho_\sigma(\boldsymbol{r}', \boldsymbol{r}) \\ & - \langle \Psi_{N;0} | \big[\hat{n}_{\sigma'}(\boldsymbol{r}'') - n_{\sigma'}(\boldsymbol{r}'')\big] \hat{\varrho}_\sigma(\boldsymbol{r}', \boldsymbol{r}) | \Psi_{N;0} \rangle. \end{aligned} \tag{F109}$$

Replacing $\hat{\varrho}_\sigma(\boldsymbol{r}', \boldsymbol{r}) := \hat{\psi}_\sigma^\dagger(\boldsymbol{r}') \hat{\psi}_\sigma(\boldsymbol{r})$ on the RHS of Eq. (F109) by $\big[\hat{\varrho}_\sigma(\boldsymbol{r}', \boldsymbol{r}) - \varrho_\sigma(\boldsymbol{r}', \boldsymbol{r})\big]$ does *not* lead to any quantitative change; however, it renders $\mathcal{B}_\sigma(\boldsymbol{r}, \boldsymbol{r})$ a similar *appearance* as $\mathcal{A}(\boldsymbol{r}, \boldsymbol{r})$ in Eq. (F2). This observation is relevant in that it shows that all our earlier considerations in this Appendix with regard to $\mathcal{A}'(\boldsymbol{r},\boldsymbol{r})$ corresponding to uniform and isotropic GSs directly apply to the regularized counterpart of $\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r})$ corresponding to these systems.

From Eqs. (B29) and (F109) we obtain

$$\mathcal{B}_\sigma(\boldsymbol{r},\boldsymbol{r}') = v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) - v_H(\boldsymbol{r};[n])\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) + \mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}') \qquad \text{(F110)}$$

where

$$\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}') := -\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'') \times \sum_{\sigma'} \langle \Psi_{N;0}|\big[\hat{n}_{\sigma'}(\boldsymbol{r}'') - n_{\sigma'}(\boldsymbol{r}'')\big]\hat{\varrho}_\sigma(\boldsymbol{r}',\boldsymbol{r})|\Psi_{N;0}\rangle. \quad \text{(F111)}$$

Since the integral with respect to $\boldsymbol{r}''$ of the GS expectation value on the RHS of Eq. (F111) is identically vanishing (compare with Eq. (F5) above), it follows that, for a constant v, $\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}') \equiv 0$. Consequently, when $v \equiv v_c$, $\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ decreases *faster* than $1/\|\boldsymbol{r}\|$ for $\|\boldsymbol{r}\| \to \infty$. This is established through invoking on the RHS of Eq. (F111) the multipole expansion for $v_c(\boldsymbol{r}-\boldsymbol{r}'')$ as presented in Eq. (F20).

In practice, where one calculates $\Gamma^{(m)}$, $m = 1,2,\dots$, evaluation of $\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ according to the expression in Eq. (F111) is not useful. A useful expression is obtained by employing Eq. (F110) as the *defining* expression for $\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$. One readily obtains

$$\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}') = -v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) - \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'') \sum_{\sigma'} \Big\{ \Gamma^{(2)}(\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}'\sigma,\boldsymbol{r}''\sigma') - n_{\sigma'}(\boldsymbol{r}'')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \Big\}. \quad \text{(F112)}$$

In order to facilitate notation in the main text, we introduce

$$\mathcal{B}''_\sigma(\boldsymbol{r},\boldsymbol{r}') := \mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}') + v(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}). \qquad \text{(F113)}$$

For completeness, within the framework of the SSDA we have (see Eq. (C6))

$$\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')\big|_{\mathrm{s}} = -v(\boldsymbol{r}-\boldsymbol{r}')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}',\boldsymbol{r}) + \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}',\boldsymbol{r}'')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}'',\boldsymbol{r}). \quad \text{(F114)}$$

For $v \equiv v_c$, owing to the idempotency of the Slater-Fock density matrices, the leading term in the AS of the integral on the RHS of Eq. (F114) for $\|\boldsymbol{r}\| \to \infty$ is equal to [134] $v_c(\boldsymbol{r})\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}',\boldsymbol{r}) \sim v_c(\boldsymbol{r}-\boldsymbol{r}')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}',\boldsymbol{r})$, where we have assumed $\|\boldsymbol{r}'\|$ to be finite. This contribution cancels the first term on the RHS of Eq. (F114), implying that, similar to the *exact* $\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$, the approximation in Eq. (F114) decays *faster* than $1/\|\boldsymbol{r}\|$ for $\|\boldsymbol{r}\| \to \infty$.

3. $\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and its regularized forms $\mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and $\mathcal{G}''_\sigma(\boldsymbol{r},\boldsymbol{r}')$

Making use of the anticommutation relations in Eq. (29), from the defining equation for $\Gamma^{(3)}$ in Eq. (B1) we obtain

$$\begin{aligned}
&\Gamma^{(3)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''_1\sigma'_1,\boldsymbol{r}''_2\sigma'_2;\boldsymbol{r}\sigma,\boldsymbol{r}''_1\sigma'_1,\boldsymbol{r}''_2\sigma'_2)\\
&\quad = -\delta_{\sigma'_1,\sigma'_2}\delta(\boldsymbol{r}''_1-\boldsymbol{r}''_2)\Gamma^{(2)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''_1\sigma'_1;\boldsymbol{r}\sigma,\boldsymbol{r}''_1\sigma'_1)\\
&\qquad +\delta_{\sigma,\sigma'_1}\delta_{\sigma,\sigma'_2}\delta(\boldsymbol{r}'-\boldsymbol{r}''_1)\delta(\boldsymbol{r}-\boldsymbol{r}''_2)\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\\
&\qquad -\delta_{\sigma,\sigma'_1}\delta(\boldsymbol{r}'-\boldsymbol{r}''_1)\,\langle\Psi_{N;0}|\hat{\varrho}_\sigma(\boldsymbol{r}',\boldsymbol{r})\hat{n}_{\sigma'_2}(\boldsymbol{r}''_2)|\Psi_{N;0}\rangle\\
&\qquad -\delta_{\sigma,\sigma'_2}\delta(\boldsymbol{r}'-\boldsymbol{r}''_2)\,\langle\Psi_{N;0}|\hat{n}_{\sigma'_1}(\boldsymbol{r}''_1)\hat{\varrho}_\sigma(\boldsymbol{r}',\boldsymbol{r})|\Psi_{N;0}\rangle\\
&\qquad +\langle\Psi_{N;0}|\hat{n}_{\sigma'_1}(\boldsymbol{r}''_1)\hat{n}_{\sigma'_2}(\boldsymbol{r}''_2)\hat{\varrho}_\sigma(\boldsymbol{r}',\boldsymbol{r})|\Psi_{N;0}\rangle. \qquad \text{(F115)}
\end{aligned}$$

Employing this result, Eq. (E18) can be re-written as

$$\begin{aligned}
\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}') &= v^2(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) + 2v(\boldsymbol{r}-\boldsymbol{r}')\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')\\
&\quad -2v(\boldsymbol{r}-\boldsymbol{r}')v_H(\boldsymbol{r};[n])\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) - 2v_H(\boldsymbol{r};[n])\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')\\
&\quad +v_H^2(\boldsymbol{r};[n])\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) + \mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}'), \qquad \text{(F116)}
\end{aligned}$$

where

$$\mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}') := \int \mathrm{d}^d r''_1 \mathrm{d}^d r''_2\; v(\boldsymbol{r}-\boldsymbol{r}''_1)v(\boldsymbol{r}-\boldsymbol{r}''_2) \times \sum_{\sigma'_1,\sigma'_2} \langle\Psi_{N;0}|\big[\hat{n}_{\sigma'_1}(\boldsymbol{r}''_1) - n_{\sigma'_1}(\boldsymbol{r}''_1)\big] \times\big[\hat{n}_{\sigma'_2}(\boldsymbol{r}''_2) - n_{\sigma''_2}(\boldsymbol{r}''_2)\big]\hat{\varrho}_\sigma(\boldsymbol{r}',\boldsymbol{r})|\Psi_{N;0}\rangle. \quad \text{(F117)}$$

Since $\big[\hat{n}_\sigma(\boldsymbol{r}),\hat{n}_{\sigma'}(\boldsymbol{r}')\big]_- = 0$, $\big[\hat{n}_{\sigma'_2}(\boldsymbol{r}''_2) - n_{\sigma'_2}(\boldsymbol{r}''_2)\big]$ in the RHS of Eq. (F117) can be transposed to the left of $\big[\hat{n}_{\sigma'_1}(\boldsymbol{r}''_1) - n_{\sigma'_1}(\boldsymbol{r}''_1)\big]$. It follows that the integrals with respect to both $\boldsymbol{r}''_1$ *and* $\boldsymbol{r}''_2$ of $\sum_{\sigma'_1,\sigma'_2}\langle\Psi_{N;0}|\dots|\Psi_{N;0}\rangle$ on the RHS of Eq. (102) are identically vanishing (*cf.* Eq. (F5); see also text following Eq. (F111) above). Thus, in the case of $d=3$ and $v \equiv v_c$, $\mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ decays more rapidly than $1/\|\boldsymbol{r}\|^2$ for $\|\boldsymbol{r}\| \to \infty$.

In the case where $d = 3$ and $v \equiv v_c$ and the system under consideration is in the thermodynamic limit, each $v_c(\boldsymbol{r}-\boldsymbol{r}')$ in the above expressions is accompanied by the appropriate smooth cut-off function $\exp(-\kappa\|\boldsymbol{r}-\boldsymbol{r}'\|)$, with $\kappa \downarrow 0$ (see Eq. (13) and the text following Eq. (15)). Here, as in other cases, the limit $\kappa \downarrow 0$ is taken *following* evaluation of the pertinent integrals over the space occupied by the system with volume $\Omega \to \infty$ (see Eq. (10)). Since under these conditions, $\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ as well as $\mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ are bounded, from Eq. (F116) and the *unboundedness* of $v_H(\boldsymbol{r};[n])$ for $\kappa \downarrow 0$, it follows that, for $v \equiv v_c$ in $d = 3$, $\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ is unbounded in the thermodynamic limit. As

[134] The LHS of this relation is deduced by employing the multipole expansion in Eq. (F20).

can be verified from Eq. (199) (see also Eqs. (210) - (212) and (214)), $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ does *not* depend on $\mathcal{G}_\sigma(\boldsymbol{r},\boldsymbol{r}')$, but only on $\mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$, nor does $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ depend on $v_H(\boldsymbol{r};[n])$ but on $v_H(\boldsymbol{r};[n'])$, which is bounded in the thermodynamic limit.

The expression for $\mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (F117) is not useful for the purpose of actual calculations where the correlation functions $\Gamma^{(m)}$ are the basic functions. Taking Eq. (F116) as the defining equation for $\mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$, some elementary algebra yields

$$\begin{aligned}
\mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}') &= \int \mathrm{d}^d r''_1\; v(\boldsymbol{r}-\boldsymbol{r}''_1)\Big(v(\boldsymbol{r}-\boldsymbol{r}''_1)\\
&\times \sum_{\sigma'} \Big[\Gamma^{(2)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''_1\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}''_1\sigma'_1) - n_{\sigma'}(\boldsymbol{r}''_1)\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\Big]\\
&+\int \mathrm{d}^d r''_2\; v(\boldsymbol{r}-\boldsymbol{r}''_2)\\
&\times \sum_{\sigma'_1,\sigma'_2} \Big[\Gamma^{(3)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''_1\sigma'_1,\boldsymbol{r}''_2\sigma''_2;\boldsymbol{r}\sigma,\boldsymbol{r}''_1\sigma'_1,\boldsymbol{r}''_2\sigma'_2)\\
&\qquad - n_{\sigma'_1}(\boldsymbol{r}''_1)n_{\sigma'_2}(\boldsymbol{r}''_2)\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\Big]\\
&+\sum_{\sigma'} n_{\sigma'}(\boldsymbol{r}''_1)\Big[\big\{2v(\boldsymbol{r}-\boldsymbol{r}')+v(\boldsymbol{r}-\boldsymbol{r}''_1)\big\}\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\\
&\qquad +2\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')\Big]\Big)\\
&-v^2(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) - 2v(\boldsymbol{r}-\boldsymbol{r}')\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}'). \qquad \text{(F118)}
\end{aligned}$$

In order to facilitate notation in the main text, noting from Eq. (F113) that $-v^2\varrho_\sigma - 2v\mathcal{B}'_\sigma = v^2\varrho_\sigma - 2v\mathcal{B}''_\sigma$, we introduce

$$\mathcal{G}''_\sigma(\boldsymbol{r},\boldsymbol{r}') := \mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}') - v^2(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}). \qquad \text{(F119)}$$

Finally, within the framework of the SSDA (see Appendix C) we have

$$\begin{aligned}
\mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}')\vert_{\mathrm{s}} &= \mathcal{A}'_{\mathrm{s}}(\boldsymbol{r},\boldsymbol{r})\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}',\boldsymbol{r})\\
&-\int \mathrm{d}^d r''\; v^2(\boldsymbol{r}-\boldsymbol{r}'')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}',\boldsymbol{r}'')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}'',\boldsymbol{r})\\
&+2\int \mathrm{d}^d r''_1 \mathrm{d}^d r''_2\; v(\boldsymbol{r}-\boldsymbol{r}''_1)v(\boldsymbol{r}-\boldsymbol{r}''_2)\\
&\qquad \times \varrho_{\mathrm{s};\sigma}(\boldsymbol{r}',\boldsymbol{r}''_1)\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}''_1,\boldsymbol{r}''_2)\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}''_2,\boldsymbol{r})\\
&-v^2(\boldsymbol{r}-\boldsymbol{r}')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}',\boldsymbol{r}) - 2v(\boldsymbol{r}-\boldsymbol{r}')\mathcal{B}'_{\mathrm{s};\sigma}(\boldsymbol{r},\boldsymbol{r}'). \qquad \text{(F120)}
\end{aligned}$$

4. $\mathcal{K}_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and its regularized forms $\mathcal{K}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$, $\mathcal{K}''_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and $\mathcal{K}'''_\sigma(\boldsymbol{r},\boldsymbol{r}')$

In the expression for $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ in Eq. (199) we encounter

$$\begin{aligned}
\mathcal{K}_\sigma(\boldsymbol{r},\boldsymbol{r}') &:= \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\\
&\times \sum_{\sigma'} \Gamma^{(2)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma')\\
&+\int \mathrm{d}^d r''_1 \mathrm{d}^d r''_2\; v(\boldsymbol{r}-\boldsymbol{r}''_1)v(\boldsymbol{r}'-\boldsymbol{r}''_2)\\
&\times \sum_{\sigma'_1,\sigma'_2} \Gamma^{(3)}(\boldsymbol{r}'\sigma,\boldsymbol{r}''_1\sigma'_1,\boldsymbol{r}''_2\sigma'_2;\boldsymbol{r}\sigma,\boldsymbol{r}''_1\sigma'_1,\boldsymbol{r}''_2\sigma'_2), \qquad \text{(F121)}
\end{aligned}$$

which, like $\mathcal{A}'(\boldsymbol{r},\boldsymbol{r}')$ but unlike $\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and $\mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$, *is* symmetric with respect to $\boldsymbol{r} \rightleftharpoons \boldsymbol{r}'$. Making use of the expression in Eq. (F115) together with the commutation relation

$$\big[\hat{n}_{\sigma'}(\boldsymbol{r}''),\hat{\varrho}_\sigma(\boldsymbol{r}',\boldsymbol{r})\big]_- = \delta_{\sigma,\sigma'}\big\{\delta(\boldsymbol{r}'-\boldsymbol{r}'')-\delta(\boldsymbol{r}-\boldsymbol{r}'')\big\} \times\hat{\varrho}_\sigma(\boldsymbol{r}',\boldsymbol{r}), \qquad \text{(F122)}$$

we obtain

$$\begin{aligned}
\mathcal{K}_\sigma(\boldsymbol{r},\boldsymbol{r}') &= \Big\{v^2(\boldsymbol{r}-\boldsymbol{r}') + v_H(\boldsymbol{r};[n])v_H(\boldsymbol{r}';[n])\\
&\qquad -v(\boldsymbol{r}-\boldsymbol{r}')\big[v_H(\boldsymbol{r};[n])+v_H(\boldsymbol{r}';[n])\big]\Big\}\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\\
&+v(\boldsymbol{r}-\boldsymbol{r}')\big[\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')+\mathcal{B}'_\sigma(\boldsymbol{r}',\boldsymbol{r})\big]\\
&-v_H(\boldsymbol{r};[n])\mathcal{B}'_\sigma(\boldsymbol{r}',\boldsymbol{r}) - v_H(\boldsymbol{r}';[n])\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}') + \mathcal{K}'_\sigma(\boldsymbol{r},\boldsymbol{r}'), \qquad \text{(F123)}
\end{aligned}$$

where

$$\begin{aligned}
\mathcal{K}'_\sigma(\boldsymbol{r},\boldsymbol{r}') &:= \int \mathrm{d}^d r''_1 \mathrm{d}^d r''_2\; v(\boldsymbol{r}-\boldsymbol{r}''_1)v(\boldsymbol{r}'-\boldsymbol{r}''_2)\\
&\times \sum_{\sigma'_1,\sigma'_2} \langle\Psi_{N;0}\vert\big[\hat{n}_{\sigma'_1}(\boldsymbol{r}''_1)-n_{\sigma'_1}(\boldsymbol{r}''_1)\big]\hat{\varrho}_\sigma(\boldsymbol{r}',\boldsymbol{r})\\
&\qquad \times\big[\hat{n}_{\sigma'_2}(\boldsymbol{r}''_2)-n_{\sigma'_2}(\boldsymbol{r}''_2)\big]\vert\Psi_{N;0}\rangle. \qquad \text{(F124)}
\end{aligned}$$

It is easily verified that the integrals with respect to $\boldsymbol{r}''_1$ and $\boldsymbol{r}''_2$ of $\sum_{\sigma'_1,\sigma'_2}\langle\Psi_{N;0}\vert\dots\vert\Psi_{N;0}\rangle$ on the RHS of Eq. (F124) are identically vanishing (compare with functions of similar characteristic property encountered in dealing with $\mathcal{A}'(\boldsymbol{r},\boldsymbol{r}')$, $\mathcal{B}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ and $\mathcal{G}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$).

For uniform and isotropic GSs, $\mathcal{K}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ is a function of $\Vert\boldsymbol{r}-\boldsymbol{r}'\Vert$ and for the reason that the integrals with respect to $\boldsymbol{r}''_1$ and $\boldsymbol{r}''_2$ of $\sum_{\sigma'_1,\sigma'_2}\langle\Psi_{N;0}\vert\dots\vert\Psi_{N;0}\rangle$ on the RHS of Eq. (F124) are vanishing, it decays *more rapidly* than $1/\Vert\boldsymbol{r}-\boldsymbol{r}'\Vert$ for $\Vert\boldsymbol{r}-\boldsymbol{r}'\Vert\to\infty$. For non-uniform systems, $\mathcal{K}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ decreases *more rapidly* than $1/\Vert\boldsymbol{r}\Vert$ and $1/\Vert\boldsymbol{r}'\Vert$ for $\Vert\boldsymbol{r}\Vert,\Vert\boldsymbol{r}'\Vert\to\infty$. In arriving at these conclusions we have relied upon the multipole series expansion in Eq. (F20) above.

Similar to the other functions that we have dealt with thus far in this Appendix, $\mathcal{K}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ according to its defining expression in Eq. (F124) is *not* amenable to direct numerical calculation. In contrast, the following expression, which one obtains through employing Eq. (F123) as the defining expression for $\mathcal{K}'_\sigma(\boldsymbol{r},\boldsymbol{r}')$ followed by judiciously rearranging terms, is readily verified to be suitable for direct numerical evaluation:

$$\begin{aligned}
\mathcal{K}'_\sigma(\boldsymbol{r},\boldsymbol{r}') &= v^2(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})\\
&-v(\boldsymbol{r}-\boldsymbol{r}')\big[\mathcal{B}''_\sigma(\boldsymbol{r},\boldsymbol{r}')+\mathcal{B}''_\sigma(\boldsymbol{r}',\boldsymbol{r})\big]
\end{aligned}$$

$$+\int \mathrm{d}^d r_1''\, v(\boldsymbol{r}-\boldsymbol{r}_1'')\Big(v(\boldsymbol{r}'-\boldsymbol{r}_1'')$$
$$\times \sum_{\sigma_1'} \Gamma^{(2)}(\boldsymbol{r}'\sigma, \boldsymbol{r}_1''\sigma_1'; \boldsymbol{r}\sigma, \boldsymbol{r}_1''\sigma_1')$$
$$+\int \mathrm{d}^d r_2''\, v(\boldsymbol{r}'-\boldsymbol{r}_2'') \sum_{\sigma_1',\sigma_2'}$$
$$\times\Big[\Gamma^{(3)}(\boldsymbol{r}'\sigma, \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'; \boldsymbol{r}\sigma, \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2')$$
$$-n_{\sigma_1'}(\boldsymbol{r}_1'')\Gamma^{(2)}(\boldsymbol{r}\sigma, \boldsymbol{r}_2''\sigma_2''; \boldsymbol{r}'\sigma, \boldsymbol{r}_2''\sigma_2'')$$
$$-n_{\sigma_2'}(\boldsymbol{r}_2'')\Gamma^{(2)}(\boldsymbol{r}'\sigma, \boldsymbol{r}_1''\sigma_1''; \boldsymbol{r}\sigma, \boldsymbol{r}_1''\sigma_1'')$$
$$+n_{\sigma_1'}(\boldsymbol{r}_1'')n_{\sigma_2'}(\boldsymbol{r}_2'')\varrho_\sigma(\boldsymbol{r}', \boldsymbol{r})\Big]\Big). \qquad \text{(F125)}$$

It can be verified that the $\boldsymbol{r}_1''$ and $\boldsymbol{r}_2''$ integrals on the RHS of Eq. (F125) are bounded for $d = 3$ and $v \equiv v_c$. This aspect crucially depends on the specific way in which various terms are combined in Eq. (F125), signified by means of large parentheses and square brackets. It is therefore crucial that in particular in the case of $d = 3$ and $v \equiv v_c$, the structure of the expression in Eq. (F125) is adhered to as closely as possible.

We introduce

$$\mathcal{K}_\sigma''(\boldsymbol{r}, \boldsymbol{r}') {:=} \mathcal{K}_\sigma'(\boldsymbol{r}, \boldsymbol{r}') - v^2(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}', \boldsymbol{r}). \qquad \text{(F126)}$$

It is further useful to define

$$\mathcal{K}_\sigma'''(\boldsymbol{r}, \boldsymbol{r}') {:=} \mathcal{K}_\sigma''(\boldsymbol{r}, \boldsymbol{r}') + v(\boldsymbol{r}-\boldsymbol{r}')\big[\mathcal{B}_\sigma''(\boldsymbol{r}, \boldsymbol{r}') + \mathcal{B}_\sigma''(\boldsymbol{r}', \boldsymbol{r})\big]. \qquad \text{(F127)}$$

This enables us to take full account of a contribution to $\widetilde{\Sigma}_{\sigma;\infty_2}(\boldsymbol{r}, \boldsymbol{r}'|z)$, namely $\Sigma^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{r}, \boldsymbol{r}')$ (see Eqs. (210) and (212)), that is bounded almost everywhere; however, it is *not* integrable (see criteria (A)-(C) in § II.B).

Finally, within the framework of the SSDA (see Appendix C) we have

$$\mathcal{K}_\sigma'(\boldsymbol{r}, \boldsymbol{r}')|_{\mathrm{s}} = v^2(\boldsymbol{r}-\boldsymbol{r}')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}', \boldsymbol{r})$$
$$-v(\boldsymbol{r}-\boldsymbol{r}')\big[\mathcal{B}_{\mathrm{s};\sigma}''(\boldsymbol{r}, \boldsymbol{r}') + \mathcal{B}_{\mathrm{s};\sigma}''(\boldsymbol{r}', \boldsymbol{r})\big]$$
$$+\int \mathrm{d}^d r_1''\, v(\boldsymbol{r}-\boldsymbol{r}_1'')\Big(v(\boldsymbol{r}'-\boldsymbol{r}_1'')\sum_{\sigma'} n_{\sigma'}(\boldsymbol{r}_1'')$$
$$-\int \mathrm{d}^d r_2''\, v(\boldsymbol{r}'-\boldsymbol{r}_2'')\sum_{\sigma'} \varrho^2_{\mathrm{s};\sigma'}(\boldsymbol{r}_1'', \boldsymbol{r}_2'')\Big)\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}', \boldsymbol{r})$$
$$-\int \mathrm{d}^d r''\, v(\boldsymbol{r}-\boldsymbol{r}'')v(\boldsymbol{r}'-\boldsymbol{r}'')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}', \boldsymbol{r}'')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}'', \boldsymbol{r})$$
$$+2\int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\, v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}'-\boldsymbol{r}_2'')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}', \boldsymbol{r}_1'')$$
$$\times\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}_1'', \boldsymbol{r}_2'')\varrho_{\mathrm{s};\sigma}(\boldsymbol{r}_2'', \boldsymbol{r}). \qquad \text{(F128)}$$

5. $\mathcal{L}(\boldsymbol{r})$ and its regularized form

a. Basic considerations; $\mathcal{L}'(\boldsymbol{r})$, $\mathcal{L}''(\boldsymbol{r})$, $\mathcal{M}(\boldsymbol{r})$ and $\widetilde{\mathsf{M}}(\boldsymbol{r};z)$

In the expression for $\Sigma_{\sigma;\infty_2}(\boldsymbol{r}, \boldsymbol{r}')$ in Eq. (199) we encounter

$$\mathcal{L}(\boldsymbol{r}) {:=} \int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\mathrm{d}^d r_3''\, v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_2'')v(\boldsymbol{r}-\boldsymbol{r}_3'')$$
$$\times \sum_{\sigma_1',\sigma_2',\sigma_3'} \Gamma^{(3)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2', \boldsymbol{r}_3''\sigma_3'; \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2', \boldsymbol{r}_3''\sigma_3') \qquad \text{(F129)}$$

which, making use of the definition for $\Gamma^{(3)}$ in Eq. (B1) and the anticommutation relations in Eq. (29), can be put into the following form:

$$\mathcal{L}(\boldsymbol{r}) = 2\int \mathrm{d}^d r''\, v^3(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')$$
$$-3v_H(\boldsymbol{r};[n])\int \mathrm{d}^d r''\, v^2(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')$$
$$-3\int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\, v^2(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_2'')\mathcal{U}(\boldsymbol{r}_1'', \boldsymbol{r}_2'')$$
$$+3v_H(\boldsymbol{r};[n])\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}) + v_H^3(\boldsymbol{r};[n]) + \mathcal{L}'(\boldsymbol{r}), \qquad \text{(F130)}$$

where $\mathcal{U}(\boldsymbol{r}_1'', \boldsymbol{r}_2'')$ and $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r})$ are defined in Eqs. (F4) and (F3) respectively, and

$$\mathcal{L}'(\boldsymbol{r}) {:=} \int \mathrm{d}^d r_1''\mathrm{d}^d r_2''\mathrm{d}^d r_3''\, v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_2'')v(\boldsymbol{r}-\boldsymbol{r}_3'')$$
$$\times \sum_{\sigma_1',\sigma_2',\sigma_3'} \langle\Psi_{N;0}|\big[\hat{n}_{\sigma_1'}(\boldsymbol{r}_1'') - n_{\sigma_1'}(\boldsymbol{r}_1'')\big]$$
$$\times\big[\hat{n}_{\sigma_2'}(\boldsymbol{r}_2'') - n_{\sigma_2'}(\boldsymbol{r}_2'')\big]$$
$$\times\big[\hat{n}_{\sigma_3'}(\boldsymbol{r}_3'') - n_{\sigma_3'}(\boldsymbol{r}_3'')\big]|\Psi_{N;0}\rangle. \qquad \text{(F131)}$$

The similarity of this to other (singly-primed) functions, such as $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$, $\mathcal{B}_\sigma'(\boldsymbol{r}, \boldsymbol{r}')$ in Eqs. (F3) and (F111) respectively, is suggestive of $\mathcal{L}'(\boldsymbol{r})$ being bounded for $v \equiv v_c$ in $d = 3$. For the reasons that we shall present shortly, this is *not* the case however. For now, we point out that $\mathcal{L}'(\boldsymbol{r})$ similar to $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ and $\mathcal{B}_\sigma'(\boldsymbol{r}, \boldsymbol{r}')$ does *not* suffer from the consequences of the long range of the Coulomb potential; it rather suffers from the singular behaviour of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ for $\|\boldsymbol{r}-\boldsymbol{r}'\| \to 0$ (this is similar to the situation with regard to $\mathcal{A}'(\boldsymbol{r}, \boldsymbol{r}')$ in $d = 2$ (B. Farid, 2001, unpublished)). It is not difficult to demonstrate that this behaviour of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ is of considerable consequence not only to $\Sigma_{\sigma;\infty_2}(\boldsymbol{r}, \boldsymbol{r}')$ but also to $\Sigma_{\sigma;\infty_m}(\boldsymbol{r}, \boldsymbol{r}')$ for *all* $m \geq 2$ (here $m = 2$ is specific to $d = 3$).

Before discussing the behaviour of $\mathcal{L}'(\boldsymbol{r})$ for the specific case corresponding to $v \equiv v_c$ in $d = 3$, on employing Eq. (F130) as the defining expression for $\mathcal{L}'(\boldsymbol{r})$ we obtain the following expression which is suitable for direct calculation in terms of $\Gamma^{(m)}$:

$$\mathcal{L}'(\boldsymbol{r}) \equiv \mathcal{M}(\boldsymbol{r}) + \mathcal{L}''(\boldsymbol{r}), \tag{F132}$$

where (see Eq. (214))

$$\mathcal{M}(\boldsymbol{r}) := \int \mathrm{d}^d r_1''\; v^2(\boldsymbol{r}-\boldsymbol{r}_1'')\Big\{v(\boldsymbol{r}-\boldsymbol{r}_1'')n(\boldsymbol{r}_1'') + \Lambda(\boldsymbol{r}_1'',\boldsymbol{r})\Big\}, \tag{F133}$$

in which

$$\Lambda(\boldsymbol{r}_1'',\boldsymbol{r}) := -\int \mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_2'')\,\rho(\boldsymbol{r}_2'',\boldsymbol{r}_1''), \tag{F134}$$

with $\rho(\boldsymbol{r}_2'',\boldsymbol{r}_1'')$ as defined in Eq. (F13), and

$$\begin{aligned}\mathcal{L}''(\boldsymbol{r}) := &-2\int \mathrm{d}^d r_1'' \mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_2'')\\ &\times\Big\{v(\boldsymbol{r}-\boldsymbol{r}_1'')\,\rho(\boldsymbol{r}_2'',\boldsymbol{r}_1'')\\ &-\frac{1}{2}\int \mathrm{d}^d r_3''\; v(\boldsymbol{r}-\boldsymbol{r}_3'')\,\Big[3\rho(\boldsymbol{r}_2'',\boldsymbol{r}_1'')\,n(\boldsymbol{r}_3'')\\ &+\sum_{\sigma_1',\sigma_2',\sigma_3'}\Big(\Gamma^{(3)}(\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2',\boldsymbol{r}_3''\sigma_3';\boldsymbol{r}_1''\sigma_1',\boldsymbol{r}_2''\sigma_2',\boldsymbol{r}_3''\sigma_3')\\ &-n_{\sigma_1'}(\boldsymbol{r}_1'')n_{\sigma_2'}(\boldsymbol{r}_2'')n_{\sigma_3'}(\boldsymbol{r}_3'')\Big)\Big]\Big\}.\end{aligned} \tag{F135}$$

For uniform GSs, $\mathcal{L}(\boldsymbol{r})$ and its constituent parts $\mathcal{L}'(\boldsymbol{r})$, $\mathcal{M}(\boldsymbol{r})$ and $\mathcal{L}''(\boldsymbol{r})$ do *not* depend on $\boldsymbol{r}$. This can be readily verified by means of shift transformations of the integration variables in the defining expressions of these functions.

Within the framework of the SSDA (see Appendix C), we have (*cf.* Eq. (F132))

$$\mathcal{L}_{\mathrm{s}}'(\boldsymbol{r}) \equiv \mathcal{M}_{\mathrm{s}}(\boldsymbol{r}) + \mathcal{L}_{\mathrm{s}}''(\boldsymbol{r}), \tag{F136}$$

where

$$\begin{aligned}\mathcal{M}_{\mathrm{s}}(\boldsymbol{r}) \equiv \int \mathrm{d}^d r_1''\; v^2(\boldsymbol{r}-\boldsymbol{r}_1'')\Big\{&v(\boldsymbol{r}-\boldsymbol{r}_1'')n_{\mathrm{s}}(\boldsymbol{r}_1'')\\ &+\Lambda_{\mathrm{s}}(\boldsymbol{r}_1'',\boldsymbol{r})\Big\},\end{aligned} \tag{F137}$$

in which (*cf.* Eqs. (F134) and (F135))

$$\Lambda_{\mathrm{s}}(\boldsymbol{r}_1'',\boldsymbol{r}) \equiv -\int \mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_2'')\,\rho_{\mathrm{s}}(\boldsymbol{r}_2'',\boldsymbol{r}_1''), \tag{F138}$$

and

$$\begin{aligned}\mathcal{L}_{\mathrm{s}}''(\boldsymbol{r}) \equiv &-2\int \mathrm{d}^d r_1'' \mathrm{d}^d r_2''\; v(\boldsymbol{r}-\boldsymbol{r}_1'')v(\boldsymbol{r}-\boldsymbol{r}_2'')\\ &\times\Big\{v(\boldsymbol{r}-\boldsymbol{r}_1'')\rho_{\mathrm{s}}(\boldsymbol{r}_1'',\boldsymbol{r}_2'')\\ &-\int \mathrm{d}^d r_3''\; v(\boldsymbol{r}-\boldsymbol{r}_3'')\sum_{\sigma'}\varrho_{\mathrm{s};\sigma'}(\boldsymbol{r}_1'',\boldsymbol{r}_2'')\\ &\times\varrho_{\mathrm{s};\sigma'}(\boldsymbol{r}_2'',\boldsymbol{r}_3'')\varrho_{\mathrm{s};\sigma'}(\boldsymbol{r}_3'',\boldsymbol{r}_1'')\Big\},\end{aligned} \tag{F139}$$

where $\rho_{\mathrm{s}}(\boldsymbol{r}_1'',\boldsymbol{r}_2'') \equiv \sum_{\sigma'}\varrho_{\mathrm{s};\sigma'}^2(\boldsymbol{r}_1'',\boldsymbol{r}_2'')$ (see Eq. (F13) above and the subsequent text).

It can be shown that $\mathcal{L}''(\boldsymbol{r})$ is a well-defined and bounded function of $\boldsymbol{r}$, a fact that can be readily verified through examining $\mathcal{L}_{\mathrm{s}}''(\boldsymbol{r})$, taking into account the simplifying aspect associated with the idempotency of $\varrho_{\mathrm{s};\sigma}$.

The analysis of the exact $\mathcal{M}(\boldsymbol{r})$ is facilitated by first considering $\mathcal{M}_{\mathrm{s}}(\boldsymbol{r})$ in Eq. (F137). To this end we first point out that in the case of $v \equiv v_c$ in $d=3$, [135]

$$\Lambda_{\mathrm{s}}(\boldsymbol{r}_1'',\boldsymbol{r}) \sim -v_c(\boldsymbol{r}-\boldsymbol{r}_1'')\,n_{\mathrm{s}}(\boldsymbol{r}_1''),\;\; \|\boldsymbol{r}_1''\|\to\infty, \tag{F140}$$

so that for $\|\boldsymbol{r}_1''\|\to\infty$ the integrand of the $\boldsymbol{r}_1''$ integral on the RHS of Eq. (F133) decays *more rapidly* than $1/\|\boldsymbol{r}_1''\|^3$. Consequently, the $\boldsymbol{r}_1''$ integral is *not* infrared divergent. If there was no $v_c(\boldsymbol{r}-\boldsymbol{r}_1'')n_{\mathrm{s}}(\boldsymbol{r}_1'')$ on the RHS of Eq. (F140), the integrand of the $\boldsymbol{r}_1''$ integral on the RHS of Eq. (F137) would have decayed like $1/\|\boldsymbol{r}_1''\|^3$ and consequently this integral would have been infrared divergent. Thus a contribution of the form $\int \mathrm{d}^3 r_1''\; v_c^3(\boldsymbol{r}-\boldsymbol{r}_1'')\,n_{\mathrm{s}}(\boldsymbol{r}_1'')$ to $\mathcal{M}_{\mathrm{s}}(\boldsymbol{r})$ seems necessary. On the other hand, it is evident that the singularity of $v_c^3(\boldsymbol{r}-\boldsymbol{r}_1'')$ at $\boldsymbol{r}_1''=\boldsymbol{r}$ is *not* integrable in $d=3$. Given the fact that $\Lambda_{\mathrm{s}}(\boldsymbol{r}_1'',\boldsymbol{r})$ is bounded for $\boldsymbol{r}_1''=\boldsymbol{r}$ and that the singularity of $v_c^2(\boldsymbol{r}-\boldsymbol{r}_1'')$ at $\boldsymbol{r}_1''=\boldsymbol{r}$ *is* integrable, we observe that, in the case where $v\equiv v_c$ and $d=3$, the $\boldsymbol{r}_1''$ integral on the RHS of Eq. (F137) is *unbounded*, that is it is so-called ultraviolet divergent. An analysis along the same line (see footnote 135) demonstrates the fact that the exact $\mathcal{M}(\boldsymbol{r})$ is similar to $\mathcal{M}_{\mathrm{s}}(\boldsymbol{r})$ unbounded for $v\equiv v_c$ and $d=3$. Thus, whereas, in common with other 'primed' functions that we have considered in this Appendix, $\mathcal{L}'(\boldsymbol{r})$ through $\mathcal{M}(\boldsymbol{r})$ (see Eq. (F132)) is infrared regular (in the case $v\equiv v_c$ and $d=3$), it nevertheless is *unbounded* owing to the ultraviolet-divergent integral $\int \mathrm{d}^3 r_1''\; v_c^3(\boldsymbol{r}-\boldsymbol{r}_1'')n(\boldsymbol{r}_1'')$.

In the light of our above discussion, from the considerations in § II.B it follows that $\hbar^{-1}\mathcal{M}(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}')$ must have local counterparts pertaining to $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ with $m>2$, described by ultraviolet-divergent integrals. Indeed, it can be shown that $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ involves the

[135] The result in Eq. (F140) is easiest deduced by considering the fact that, since $\sum_{\sigma'}\varrho_{\mathrm{s};\sigma'}^2(\boldsymbol{r}_2'',\boldsymbol{r}_1'') \equiv \rho_{\mathrm{s}}(\boldsymbol{r}_2'',\boldsymbol{r}_1'')$ is a strongly decaying function for $\|\boldsymbol{r}_1''-\boldsymbol{r}_2''\|\to\infty$ (see, for example, Eq. (F69)), from which it follows that for $\|\boldsymbol{r}_1''\|\to\infty$ the most significant contribution to the integral on the RHS of Eq. (F138) originates from the $\boldsymbol{r}_2''$ integration in a close neighbourhood of $\boldsymbol{r}_1''$. Consequently, replacing $v_c(\boldsymbol{r}-\boldsymbol{r}_2'')$ by $v_c(\boldsymbol{r}-\boldsymbol{r}_1'')$, owing to the idempotency of $\varrho_{\mathrm{s};\sigma'}(\boldsymbol{r}_1'',\boldsymbol{r}_2'')$ the subsequent integration with respect to $\boldsymbol{r}_2''$ of $\sum_{\sigma'}\varrho_{\mathrm{s};\sigma'}^2(\boldsymbol{r}_1'',\boldsymbol{r}_2'')$ yields $\sum_{\sigma'} n_{\mathrm{s};\sigma'}(\boldsymbol{r}_1'') \equiv n_{\mathrm{s}}(\boldsymbol{r}_1'')$. Thus one arrives at the RHS of Eq. (F140). From Eqs. (F14) and (F134), making use of the multipole expansion in Eq. (F20), one readily deduces that similarly one has $\Lambda(\boldsymbol{r}_1'',\boldsymbol{r}) \sim -v_c(\boldsymbol{r}-\boldsymbol{r}_1'')\,n(\boldsymbol{r}_1'')$ for $\|\boldsymbol{r}_1''\|\to\infty$.

constituent local term $\hbar^{-1}\int \mathrm{d}^d r_1''\; v^m(\boldsymbol{r}-\boldsymbol{r}_1'')\,n(\boldsymbol{r}_1'')$ for $m \geq 2$. In fact, with reference to the expressions for $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')$ and $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')$ in Eqs. (174) and (185) respectively, it is readily verified that indeed

$$\frac{1}{\hbar} v_H(\boldsymbol{r};[n])\,\delta(\boldsymbol{r}-\boldsymbol{r}') \equiv \frac{1}{\hbar}\int \mathrm{d}^d r_1''\, v(\boldsymbol{r}-\boldsymbol{r}_1'')\,n(\boldsymbol{r}_1'')\delta(\boldsymbol{r}-\boldsymbol{r}')$$

is a component part of the former function and that

$$\frac{1}{\hbar}\int \mathrm{d}^d r_1''\, v^2(\boldsymbol{r}-\boldsymbol{r}_1'')\,n(\boldsymbol{r}_1'')\,\delta(\boldsymbol{r}-\boldsymbol{r}')$$

is a component part of the latter function. We thus arrive at the conclusion that (see text following Eq. (111))

$$\widetilde{\mathsf{M}}(\boldsymbol{r};z){:=}\frac{1}{z^2}\int \mathrm{d}^d r''\; v^2(\boldsymbol{r}-\boldsymbol{r}'') \times\Big(\frac{v(\boldsymbol{r}-\boldsymbol{r}'')n(\boldsymbol{r}'')}{1-v(\boldsymbol{r}-\boldsymbol{r}'')/z}+\Lambda(\boldsymbol{r}'',\boldsymbol{r})\Big) \tag{F141}$$

is the appropriate function associated with the regularization of $\mathcal{M}(\boldsymbol{r})$. For $v \equiv v_c$ in $d=3$, it is seen that, since for $\|\boldsymbol{r}-\boldsymbol{r}''\| \to \infty$ (which for finite values of $\|\boldsymbol{r}\|$ implies the condition $\|\boldsymbol{r}''\| \to \infty$) the first function enclosed by the large parentheses on the RHS of Eq. (F141) approaches $v_c(\boldsymbol{r}-\boldsymbol{r}'')\,n(\boldsymbol{r}'')$, $\widetilde{\mathsf{M}}(\boldsymbol{r};z)$ similar to $\mathcal{M}(\boldsymbol{r})$ is free from an infrared divergence; on the other hand, as it is evident, in contrast with $\mathcal{M}(\boldsymbol{r})$, $\widetilde{\mathsf{M}}(\boldsymbol{r};z)$ is *not* ultraviolet divergent. In the next Section (§ F.5.b) we explicitly consider the case corresponding to $d=3$ and $v \equiv v_c$ and calculate the leading term in the large-$|z|$ AS for $\widetilde{\mathsf{M}}(\boldsymbol{r};z)$, that is $\widetilde{\mathsf{M}}_{\infty_2}(\boldsymbol{r}|z)/z^2$, with $\widetilde{\mathsf{M}}_{\infty_2}(\boldsymbol{r}|z) \equiv \mathsf{M}^{\mathrm{r}}_{\infty_2}(\boldsymbol{r})+\widetilde{\mathsf{M}}^{\mathrm{s}}_{\infty_2}(\boldsymbol{r}\|z)$ (for our notational conventions see § III.E.2; see also footnote 31); here $\mathsf{M}^{\mathrm{r}}_{\infty_2}(\boldsymbol{r})$ is a regular function, independent of z, and $\widetilde{\mathsf{M}}^{\mathrm{s}}_{\infty_2}(\boldsymbol{r}\|z)$ in contrast diverges logarithmically as $|z| \to \infty$ (see Eqs. (F159) and (F160) below). In § II.B we have in detail discussed the principles underlying the appearance of transcendental functions of z in the regularized coefficients corresponding to the large-$|z|$ AS for $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ and therefore will not elaborate on these here.

b. The large-$|z|$ AS for $\widetilde{\mathsf{M}}(\boldsymbol{r};z)$; $\widetilde{\mathsf{M}}_{\infty_2}(\boldsymbol{r}|z)$, $\mathsf{M}^{\mathrm{r}}_{\infty_2}(\boldsymbol{r})$ and $\widetilde{\mathsf{M}}^{\mathrm{s}}_{\infty_2}(\boldsymbol{r}\|z)$

Here we consider the case where $d=3$ and $v \equiv v_c$. By shifting the origin of integration and some evident algebraic manipulations, from Eq. (F141) we deduce

$$\begin{aligned}\widetilde{\mathsf{M}}(\boldsymbol{r};z) \equiv \frac{1}{z^2}\Big[&\int_{\Omega_R} \mathrm{d}^3 r''\; v_c^2(\boldsymbol{r}'')\Lambda(\boldsymbol{r}-\boldsymbol{r}'',\boldsymbol{r})\\ &+\int_{\Omega\backslash\Omega_R} \mathrm{d}^3 r''\; v_c^2(\boldsymbol{r}'')\,\Big\{v_c(\boldsymbol{r}'')n(\boldsymbol{r}-\boldsymbol{r}'')+\Lambda(\boldsymbol{r}-\boldsymbol{r}'',\boldsymbol{r})\Big\}\\ &+\int_{\Omega_R} \mathrm{d}^3 r''\; \frac{v_c^3(\boldsymbol{r}'')n(\boldsymbol{r}-\boldsymbol{r}'')}{1-v_c(\boldsymbol{r}'')/z}\\ &+\int_{\Omega\backslash\Omega_R} \mathrm{d}^3 r''\; v_c^3(\boldsymbol{r}'')\Big\{\frac{1}{1-v_c(\boldsymbol{r}'')/z}-1\Big\}\,n(\boldsymbol{r}-\boldsymbol{r}'')\Big],\end{aligned} \tag{F142}$$

where Ω stands for the (macroscopic) volume of the system and Ω_R a spherical volume with radius R centred at the origin; $\int_{\Omega_R}$ stands for spatial integration *inside* Ω_R and $\int_{\Omega\backslash\Omega_R}$ for that *outside* Ω_R but inside Ω. In the following we assume that

$$R \gg \frac{e^2}{4\pi\epsilon_0|z|}. \tag{F143}$$

We should emphasize that, for our purpose, *any* $R > e^2/(4\pi\epsilon_0|z|)$ would suffice; however, the condition in Eq. (F143) has the advantage of reducing the complexity of the calculations to be encountered below (see text following Eq. (F153) below).

We proceed by considering the third contribution to the RHS of Eq. (F142), namely

$$\widetilde{\mathsf{S}}(\boldsymbol{r},R;z){:=}\frac{1}{z^2}\int_{\Omega_R} \mathrm{d}^3 r''\; \frac{v_c^3(\boldsymbol{r}'')n(\boldsymbol{r}-\boldsymbol{r}'')}{1-v_c(\boldsymbol{r}'')/z}. \tag{F144}$$

We assume the system under consideration to be in the thermodynamic limit and consequently adopt the decomposition of the total number density $n(\boldsymbol{r})$ in terms of n_0 and $n'(\boldsymbol{r})$ as presented in Eq. (12). In order to gain insight into the behaviour to be expected from $\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)$, we first deal with the case where $n \equiv n_0$. In this case, the integrand in the expression on the RHS of Eq. (F144) is fully isotropic so that, by employing the spherical polar coordinate system, we readily obtain (*cf.* Eq. (F155) below)

$$\begin{aligned}\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)\Big|_{n=n_0} &= \frac{4\pi}{z^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 n_0 \times\Big\{\ln\Big(R/\mathsf{a}_0-\frac{e^2}{4\pi\epsilon_0\mathsf{a}_0 z}\Big)-\ln\Big(\frac{-e^2}{4\pi\epsilon_0\mathsf{a}_0 z}\Big)\Big\}\\ &= 4\pi\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 n_0\Big\{\frac{\ln(-z/\varepsilon_0)}{z^2}+\frac{\ln(\varepsilon_0/e_R)}{z^2}\Big\} +\mathcal{O}\big(\frac{1}{z^3}\big),\end{aligned} \tag{F145}$$

where ε_0 stands for a positive constant energy, a_0 for a positive constant length and

$$e_R{:=}\frac{e^2}{4\pi\epsilon_0 R}. \tag{F146}$$

Our choice in Eq. (F143) implies that $|z|/e_R \gg 1$. In Eq. (F145), ln stands for the principal branch of the logarithm function, that is $\mathrm{Im}[\ln(z)] \in (-\pi,\pi)$.

Owing to the *linearity* of $\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)$ with respect to $n(\boldsymbol{r})$ and with reference to the result in Eq. (F145), it remains only to determine $\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)|_{n=n'}$. To this end we employ the following Fourier integral representation

$$n'(\boldsymbol{r}) = \int \frac{\mathrm{d}^3 q}{(2\pi)^3}\, \bar{n}'(\boldsymbol{q})\, \exp(i\boldsymbol{q}\cdot\boldsymbol{r}) \qquad \text{(F147)}$$

which in cases corresponding to periodic solids, can be made into a discrete Fourier series by considering $\bar{n}'(\boldsymbol{q}) = (2\pi)^3 \sum_{\boldsymbol{G}} \bar{n}'_{\boldsymbol{G}}\, \delta(\boldsymbol{q}-\boldsymbol{G})$, where the sum is over the set of reciprocal-lattice vectors corresponding to the underlying lattice. We point out that since $n'(\boldsymbol{r})$ has by definition a zero average (see Eq. (12)), $\bar{n}'(\boldsymbol{q}) \to 0$ for $\|\boldsymbol{q}\| \to 0$; in the case of periodic solids, $\bar{n}'_{\boldsymbol{G}=\boldsymbol{0}} = 0$. Further, the analytic property of $n'(\boldsymbol{r})$ in real space implies certain behaviour for $\bar{n}'(\boldsymbol{q})$ as $\|\boldsymbol{q}\| \to \infty$; as we shall discuss in some detail below (see also Appendix K), this behaviour is of important consequence to that of $\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)|_{n=n'}$ for large $|z|$.

From Eqs. (F144) and (F147), performing the $\boldsymbol{r}''$ integral in terms of the spherical polar coordinates of $\boldsymbol{r}''$, with $\boldsymbol{q}$ the polar axis, we readily obtain

$$\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)\Big|_{n=n'} = \frac{4\pi}{z^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 \times \int \frac{\mathrm{d}^3 q}{(2\pi)^3}\, \frac{\bar{n}'(\boldsymbol{q})\,\tilde{g}(\|\boldsymbol{q}\|,R;z)}{\|\boldsymbol{q}\|}\, \exp(i\boldsymbol{q}\cdot\boldsymbol{r}), \qquad \text{(F148)}$$

where [136]

$$\tilde{g}(\|\boldsymbol{q}\|,R;z) := \int_0^R \mathrm{d}r\, \frac{\sin(\|\boldsymbol{q}\|r)}{r(r-\zeta)}, \quad \zeta := \frac{e^2}{4\pi\epsilon_0 z}. \qquad \text{(F149)}$$

Following our discussions in § II.B, on general grounds (i.e. without recourse to the expressions in Eqs. (F148) and (F149)) we expect the leading asymptotic contribution to $\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)|_{n=n'}$ for $|z| \to \infty$ (i.e. $\zeta \to 0$) to be more dominant than $1/z^2$ but less so than $1/z$. This aspect is evident from the expression for $\tilde{g}(\|\boldsymbol{q}\|,R;z)$ in Eq. (F149) where, for $\zeta \to 0$ or $|z| \to \infty$, the denominator of the integrand approaches r^2, which in combination with $\sin(\|\boldsymbol{q}\|r)$ in the numerator gives rise to an integrand that diverges like $1/r$ for $r \to 0$, implying a logarithmically-divergent integral as $\zeta \to 0$. This behaviour is explicit in the expression for $\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)|_{n=n_0}$ in Eq. (F145) above.

In order to obtain the expressions for the terms in the large-$|z|$ AS for $\tilde{g}(\|\boldsymbol{q}\|,R;z)$, we first invoke the following decomposition:

$$\frac{1}{r(r-\zeta)} = -\frac{1}{\zeta}\left(\frac{1}{r} - \frac{1}{r-\zeta}\right). \qquad \text{(F150)}$$

In view of the expected behaviour of $\tilde{g}(\|\boldsymbol{q}\|,R;z)$ for $|z| \to \infty$, the contribution of $1/r$ in this fractional expansion to $\tilde{g}(\|\boldsymbol{q}\|,R;z)$ does *not* need to be considered, since $(-1/\zeta)\int_0^R \mathrm{d}r\ \sin(\|\boldsymbol{q}\|r)/r$ scales like z and therefore must be cancelled by a counter contribution in the large-$|z|$ AS for $\tilde{g}(\|\boldsymbol{q}\|,R;z)$ originating from $(-1/\zeta)(-1)/(r-\zeta)$. Indeed, in the formal series expansion for $-1/(r-\zeta) \equiv (-1/r)/(1-\zeta/r)$ around $\zeta/r = 0$, the leading term exactly cancels the $1/r$ enclosed by large parentheses on the RHS of Eq. (F150). [137] Thus, defining

$$\tilde{\mathcal{I}}(\zeta) := \int_0^R \mathrm{d}r\, \frac{\sin(\|\boldsymbol{q}\|r)}{r-\zeta}, \qquad \text{(F151)}$$

from the closed expression for $\widetilde{\mathcal{I}}(\zeta)$ we shall be able to deduce the leading term in the AS for $\tilde{g}(\|\boldsymbol{q}\|,R;z)$ corresponding to $|z| \to \infty$; we shall specify the underlying procedure for this shortly. Note the simplification achieved through replacing the need for the evaluation of the integral on the RHS of Eq. (F149) by the need to evaluate the simpler integral on the RHS of Eq. (F151).

Following the considerations in Appendix I (use the substitution $\zeta' \rightharpoonup -\zeta$ in this Appendix), assuming $\mathrm{Re}(z)\times\mathrm{Im}(z) > 0$ (i.e. z is located either in the first or in the third quadrant of the complex z plane; for some relevant details see later), we obtain (below $q \equiv \|\boldsymbol{q}\|$)

$$\begin{aligned}\tilde{\mathcal{I}}(\zeta) = &-\frac{1}{2}\sin(q\zeta)\Big[\mathrm{Ei}(iq\zeta) + \mathrm{Ei}(-iq\zeta)\Big] \\ &-\frac{i}{2}\cos(q\zeta)\Big[\mathrm{Ei}(iq\zeta) - \mathrm{Ei}(-iq\zeta)\Big] \\ &+\pi\exp(-iq\zeta)\,\Theta\big(\mathrm{Re}(z)\big) \\ &+\mathrm{Ci}\big(q(R-\zeta)\big)\sin(q\zeta) \\ &-\Big[\frac{\pi}{2} - \mathrm{Si}\big(q(R-\zeta)\big)\Big]\cos(q\zeta),\end{aligned} \qquad \text{(F152)}$$

where Ei stands for the exponential-integral function (see Appendix I), Si for the sine-integral function and Ci for the cosine-integral function (Abramowitz and Stegun 1972, pp. 231 and 232). For completeness, in arriving at the expression in Eq. (F152), we have employed the decomposition $\int_0^R \mathrm{d}r\,(\dots) = \int_0^\infty \mathrm{d}r\,(\dots) - \int_R^\infty \mathrm{d}r\,(\dots)$, the contribution of the latter integral to $\tilde{\mathcal{I}}(\zeta)$ being the last two lines on the RHS of Eq. (F152), that is those involving Ci and Si. Further, we point out that, as a consequence of the inequality in Eq. (F143), evaluation of the

[136] The condition in Eq. (F143) is equivalent to $R \gg |\zeta|$.

[137] Through Eq. (F150), the next-to-leading term in the above-mentioned expansion corresponds to a contribution of the form $1/r^2$ to $1/(r[r-\zeta])$, which, upon substitution in the RHS of Eq. (F149), gives rise to a divergent integral. This divergence signals the fact (see § II.B) that the leading term in the large-$|z|$ AS of $\tilde{g}(\|\boldsymbol{q}\|,R;z)$ is *not* a constant but a more dominant contribution. Our calculations indeed show (see Eqs. (F145) and (F155)) that this contribution scales like $\ln(-z/\varepsilon_0)$, where ε_0 stands for a positive constant energy.

integral with respect to r of $\sin(\|\boldsymbol{q}\|r)/(r-\zeta)$ over $[R,\infty)$ does *not* require the sophistication of the treatment necessary for the evaluation of the integral over $[0,R]$ (or $[0,\infty)$; see Appendix I) since, in contrast with the latter case, in the former the integral is an analytic functions of ζ in a finite neighbourhood of $\zeta=0$; this is evident from the last two contributions on the RHS of Eq. (F152) where we observe $\mathrm{Ci}\big(q(R-\zeta)\big)$ and $\mathrm{Si}\big(q(R-\zeta)\big)$ (see footnote 136).

Concerning $\mathrm{Re}(z)\times\mathrm{Im}(z)>0$, we have invoked this condition for the reason that it enables one to deduce *directly* the 'physical' $\tilde{\mathcal{I}}(\zeta)$ for real energies, that is $\mathcal{I}(e^2/[4\pi\epsilon_0\varepsilon])$; depending on whether $\varepsilon\to+\infty$ or $\varepsilon\to-\infty$, the 'physical' $\tilde{\mathcal{I}}(\zeta)$ is obtained through approaching the real ε axis from the upper half-plane and the lower half-plane respectively of the complex z plane (*cf.* Eqs. (25), (65) and (66)). We should, however, emphasize that knowledge of $\tilde{\mathcal{I}}(e^2/[4\pi\epsilon_0 z])$ in *any* open region of the z plane suffices for calculation of $\tilde{\mathcal{I}}(e^2/[4\pi\epsilon_0 z])$ in any other open region of the complex z plane through the application of the process of analytic continuation.

Let now $\mathsf{C}_{\zeta;m}\big[\tilde{f}(\zeta)\big]$ denote the coefficient of ζ^m in the *regularized* AS of $\tilde{f}(\zeta)$, with respect to the asymptotic sequence $\{1,\zeta,\zeta^2,\dots\}$, for $\zeta\to 0$; by definition, since we have to do with *regularized* AS, $\mathsf{C}_{\zeta;m}\big[\tilde{f}(\zeta)\big]$ can involve transcendental functions of ζ (see § II.B). Our above considerations have made evident that the leading asymptotic contribution to $\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)|_{n=n'}$ for $|z|\to\infty$ is determined by $\mathsf{C}_{\zeta;1}\big[\tilde{\mathcal{I}}(\zeta)\big]$. Making use of the expression in Eq. (F152) and the asymptotic expression in Eq. (I4), we obtain

$$\begin{aligned}\mathsf{C}_{\zeta;1}\big[\tilde{\mathcal{I}}(\zeta)\big] &= q\Big((\gamma-1)+\frac{1}{2}\big[\ln(iq\zeta)+\ln(-iq\zeta)\big] \\ &\quad +\pi i\Theta\big(\mathrm{Re}(z)\big)-\mathrm{Ci}(qR)+\frac{\sin(qR)}{qR}\Big) \\ &= \|\boldsymbol{q}\|\Big[(\gamma-1)+\ln(\|\boldsymbol{q}\|R)-\ln(-z/e_R) \\ &\quad -\mathrm{Ci}(\|\boldsymbol{q}\|R)+\frac{\sin(\|\boldsymbol{q}\|R)}{\|\boldsymbol{q}\|R}\Big], \qquad \text{(F153)}\end{aligned}$$

where $\gamma=0.57721\,566\dots$ stands for the Euler constant. In arriving at the last expression on the RHS of Eq. (F153) we have made use of the fact that $\big[\ln(iq\zeta)+\ln(-iq\zeta)\big]/2=\ln|q\zeta|-i\varphi$, where $\varphi=\arg(z)$ when $0\le\arg(z)<\pi/2$ and $\varphi=\pi+\arg(z)$ when $-\pi<\arg(z)\le-\pi/2$, as well as $\ln|z|+i\big(\pi+\arg(z)\big)-2\pi i\Theta\big(\mathrm{Re}(z)\big)\equiv\ln(-z)$ for $0<\arg(z)<\pi/2$ and $-\pi<\arg(z)<-\pi/2$; we have in addition invoked the condition $R\gg|\zeta|$ (see Eq. (F143) above and footnote 136), permitting us to disregard the branch cuts of Si and Ci, an aspect reflected in the following result (*cf.* Eq. (F153))

$$\begin{aligned}\mathsf{C}_{\zeta;1}\Big[\mathrm{Ci}\big(q(R-\zeta)\big)\sin(q\zeta)+\big\{\frac{\pi}{2}-\mathrm{Si}\big(q(R-\zeta)\big)\big\}\cos(q\zeta)\Big]& \\ =\mathrm{Ci}(qR)q-\sin(qR)/R.& \qquad \text{(F154)}\end{aligned}$$

Combining the above results, we eventually obtain (*cf.* Eq. (F145))

$$\begin{aligned}\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)\Big|_{n=n'} &\sim 4\pi\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 n'(\boldsymbol{r})\,\frac{\ln(-z/\varepsilon_0)}{z^2} \\ &+4\pi\left(\frac{e^2}{4\pi\epsilon_0}\right)^3\Big\{(1-\gamma)\,n'(\boldsymbol{r})+\int\frac{\mathrm{d}^3q}{(2\pi)^3}\,\bar{n}'(\boldsymbol{q}) \\ &\times\Big[\mathrm{Ci}(\|\boldsymbol{q}\|R)-\ln(\|\boldsymbol{q}\|R)-\frac{\sin(\|\boldsymbol{q}\|R)}{\|\boldsymbol{q}\|R}\Big]\exp(i\boldsymbol{q}\cdot\boldsymbol{r}) \\ &+n'(\boldsymbol{r})\ln\left(\frac{\varepsilon_0}{e_R}\right)\Big\}\frac{1}{z^2},\;\; |z|\to\infty. \qquad \text{(F155)}\end{aligned}$$

In order to verify the correctness of this result, let us assume that $\bar{n}'(\boldsymbol{q})$ in Eq. (F155) were the Fourier transform of the *total* $n(\boldsymbol{r})$ rather than that of $n'(\boldsymbol{r})$. Assuming $n(\boldsymbol{r})\equiv n_0$, we would have $\bar{n}'(\boldsymbol{q})=(2\pi)^3 n_0\delta(\boldsymbol{q})$. Making use of $\lim_{z=0}\sin(z)/z=1$ and $\mathrm{Ci}(z)\sim\gamma+\ln(z)-z^2/4+\dots$ for $z\to 0$ (see Abramowitz and Stegun 1972, p. 232), the $\boldsymbol{q}$ integral on the RHS of Eq. (F155) would identically cancel $(1-\gamma)n'(\boldsymbol{r})\equiv(1-\gamma)n_0$, thus correctly reducing the result in Eq. (F155) into that in Eq. (F145). From Eqs. (F145) and (F155) we also observe that, whereas the full total number density $n(\boldsymbol{r})$ contributes to the 'coefficient' of the $\ln(-z/e_R)/z^2$ term in the large-$|z|$ AS of $\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)$, it is only the 'fluctuating' part of $n(\boldsymbol{r})$, namely $n'(\boldsymbol{r})\equiv n(\boldsymbol{r})-n_0$ (see Eq. (12)), that contributes to the 'coefficient' of the $1/z^2$ term in this series.

In order to establish the correctness of the asymptotic result in Eq. (F155), it remains to consider the existence of the $\boldsymbol{q}$ integral on the RHS of Eq. (F155). This aspect is of utmost relevance since boundedness of this integral is not an *a priori* necessity; with reference to our considerations in § II.B, it is evident that unboundedness of this integral would signal the fact that, in a finite-order AS for $\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)$ corresponding to $|z|\to\infty$, the asymptotic term scaling like $1/z^2$ would be preceded by a more dominant term different from and in addition to $\ln(-z/\varepsilon_0)/z^2$, which is not *a priori* ruled out. The likelihood of this possibility should be the more appreciated by realizing the fact that in determining $\mathsf{C}_{\zeta;1}[\dots]$ in Eq. (F153) we have made use of AS of *transcendental* functions $\sin(\zeta')$ and $\cos(\zeta')$ (which are bounded for $\mathrm{Im}(\zeta')=0$), with $\zeta'=q\zeta$, for $\zeta'\to 0$. [138]

For establishing the existence or otherwise of the integral on the RHS of Eq. (F155), we first note that $\mathrm{Ci}(x)\sim\sin(x)/x$ for $|x|\to\infty$ (see Abramowitz and Stegun 1972, pp. 232 and 233), implying that

$$\Big(\mathrm{Ci}(\|\boldsymbol{q}\|R)-\ln(\|\boldsymbol{q}\|R)-\frac{\sin(\|\boldsymbol{q}\|R)}{\|\boldsymbol{q}\|R}\Big)\sim-\ln(\|\boldsymbol{q}\|R) \quad \text{for } \|\boldsymbol{q}\|\to\infty. \qquad \text{(F156)}$$

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[138] See footnotes 28 and 126 concerning the limitations of the Poincaré definition of AS.

In Appendix K we consider the 'smoothness' properties of $n(\boldsymbol{r})$. Here we arrive at the well-established fact that $n(\boldsymbol{r})$ possesses cusps at the positions $\{\boldsymbol{R}_j\}$ of atomic nuclei when the bare external potential $u(\boldsymbol{r})$ diverges like the Coulomb potential $v_c(\boldsymbol{r}-\boldsymbol{R}_j)$ for $\boldsymbol{r}$ approaching $\boldsymbol{R}_j$ (see Eq. (K6)). In such cases, which we consider as corresponding to the most singular of physical external potentials, $\nabla^2_{\boldsymbol{r}} n(\boldsymbol{r})$ diverges like $1/\|\boldsymbol{r}-\boldsymbol{R}_j\|$ for $\boldsymbol{r}\to\boldsymbol{R}_j$, $\forall j$ (see Eq. (K16)). This implies that, neglecting logarithmic corrections, $\bar{n}'(\boldsymbol{q})$ *cannot* decrease *more slowly* than $1/\|\boldsymbol{q}\|^4$ for $\|\boldsymbol{q}\|\to\infty$. Such asymptotic behaviour is sufficiently strongly decaying for countering the divergent behaviour of $\ln(\|\boldsymbol{q}\|R)$ for $\|\boldsymbol{q}\|\to\infty$ (see Eq. (F156) above) and securing convergence of the $\boldsymbol{q}$ integral on the RHS of Eq. (F155). We point out that the integrand of this integral is regular over the entire $\boldsymbol{q}$ space (for the behaviour of this integrand as $\|\boldsymbol{q}\|\to 0$, see text following Eq. (F155) above).

The *physical* function $\mathsf{S}(\boldsymbol{r},R;\varepsilon)$ is obtained from $\widetilde{\mathsf{S}}(\boldsymbol{r},R;z)$ through the substitution $z \rightharpoonup \varepsilon\pm i\eta$, $\eta\downarrow 0$, for $\varepsilon\to\pm\infty$. With $\mathrm{Im}\{\ln(-[\varepsilon+i\eta])\}=-\pi$ for $\varepsilon>0$ and $\mathrm{Im}\{\ln(-[\varepsilon-i\eta])\}=0$ for $\varepsilon<0$, we observe that, when $z=\varepsilon+i\eta$ with $\varepsilon>0$, the imaginary parts of the RHSs of Eqs. (F145) and (F155) are non-vanishing, decreasing like $1/\varepsilon^2$ for increasing ε, in contrast with the case corresponding to $z=\varepsilon-i\eta$ with $\varepsilon<0$ where the RHSs of Eqs. (F145) and (F155) are purely real valued. This can be easily understood by the fact that the positive definiteness of the Coulomb potential $v_c(\boldsymbol{r}'')$ implies that for $z=\varepsilon-i\eta$ and $\varepsilon<0$ the denominator of the integrand on the RHS of Eq. (F144) is never vanishing; for $z=\varepsilon+i\eta$ and $\varepsilon>0$, on the other hand, this denominator clearly changes sign in some vicinity of $\boldsymbol{r}''=\boldsymbol{0}$.

By writing (in analogy with $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ in Eq. (112))

$$\widetilde{\mathsf{M}}(\boldsymbol{r};z)\sim\frac{\widetilde{\mathsf{M}}_{\infty_2}(\boldsymbol{r}|z)}{z^2}+\dots,\quad |z|\to\infty, \tag{F157}$$

from Eqs. (F142), (F145) and (F155), employing the convention described in § III.E.2, we have (*cf.* Eq. (110))

$$\widetilde{\mathsf{M}}_{\infty_2}(\boldsymbol{r}|z)\equiv\mathsf{M}^{\mathrm{r}}_{\infty_2}(\boldsymbol{r})+\widetilde{\mathsf{M}}^{\mathrm{s}}_{\infty_2}(\boldsymbol{r}\|z), \tag{F158}$$

where (see Eq. (213))

$$\begin{aligned}\mathsf{M}^{\mathrm{r}}_{\infty_2}(\boldsymbol{r})\equiv&\int_{\Omega_R}\mathrm{d}^3r''\;v_c^2(\boldsymbol{r}'')\Lambda(\boldsymbol{r}-\boldsymbol{r}'',\boldsymbol{r})\\ &+\int_{\Omega\backslash\Omega_R}\mathrm{d}^3r''\;v_c^2(\boldsymbol{r}'')\Big\{v_c(\boldsymbol{r}'')n(\boldsymbol{r}-\boldsymbol{r}'')+\Lambda(\boldsymbol{r}-\boldsymbol{r}'',\boldsymbol{r})\Big\}\\ &+4\pi\left(\frac{e^2}{4\pi\epsilon_0}\right)^3\Big\{(1-\gamma)\,n'(\boldsymbol{r})+\int\frac{\mathrm{d}^3q}{(2\pi)^3}\,\bar{n}'(\boldsymbol{q})\\ &\times\Big[\mathrm{Ci}(\|\boldsymbol{q}\|R)-\ln(\|\boldsymbol{q}\|R)-\frac{\sin(\|\boldsymbol{q}\|R)}{\|\boldsymbol{q}\|R}\Big]\,\exp(i\boldsymbol{q}\cdot\boldsymbol{r})\\ &+n(\boldsymbol{r})\,\ln\left(\frac{\varepsilon_0}{e_R}\right)\Big\},\end{aligned} \tag{F159}$$

and (see Eq. (213))

$$\widetilde{\mathsf{M}}^{\mathrm{s}}_{\infty_2}(\boldsymbol{r}\|z)\equiv 4\pi\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 n(\boldsymbol{r})\,\ln\left(\frac{-z}{\varepsilon_0}\right). \tag{F160}$$

It is important to note that the leading-order contribution to $\widetilde{\mathsf{M}}(\boldsymbol{r};z)$ of the last term on the RHS of Eq. (F142) scales like $1/z^3$ for $|z|\to\infty$ when $R>e^2/(4\pi\epsilon_0|z|)$ so that, on account of our implicit assumption in Eq. (F143), there is no contribution to $\widetilde{\mathsf{M}}_{\infty_2}(\boldsymbol{r}|z)$ in Eq. (F158) arising from the above-mentioned term on the RHS of Eq. (F142).

Finally, in § III.I.2 we require the leading-order imaginary part of $\widetilde{\mathsf{M}}(\boldsymbol{r};z)$ for $z=\varepsilon\pm i\eta$, $\eta\downarrow 0$, as $\varepsilon\to\pm\infty$; with reference to Eq. (F157), from Eqs. (F158) - (F160) we readily obtain (*cf.* Eq. (G17)) [139]

$$\mathrm{Im}[\mathsf{M}(\boldsymbol{r};\varepsilon)]\sim-4\pi^2\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 n(\boldsymbol{r})\,\frac{\Theta(\varepsilon)}{\varepsilon^2},\quad |\varepsilon|\to\infty. \tag{F161}$$

We note in passing that by introducing the *local* Wigner-Seitz radius, namely (*cf.* Eq. (93)) [140]

$$r_0(\boldsymbol{r}){:=}\left(\frac{3}{4\pi n(\boldsymbol{r})}\right)^{1/3}, \tag{F162}$$

the coefficient of $\ln(-z/\varepsilon_0)$ in Eq. (F160), that is $3\big(e^2/[4\pi\epsilon_0 r_0(\boldsymbol{r})]\big)^3$, is seen to be equal to three times the third power of the Coulomb repulsion energy due to two particles of equal charge (either $-e$ or $+e$) at distance r_0 whose value depends on $\boldsymbol{r}$. □

APPENDIX G: REGULARIZATION OF $\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})$ AND THE LARGE-$|z|$ ASYMPTOTIC SERIES FOR $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$ ($\mathsf{T}^{\mathrm{r}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r})$, $\mathsf{T}^{\mathrm{s_b}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r})$ AND $\widetilde{\mathsf{T}}^{\mathrm{s}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}\|z)$)

In the expression for the *exact* $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ corresponding to $v\equiv v_c$ in $d=3$ we encounter the local contribution $\hbar^{-1}\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}')$ with $\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})$ as presented in Eq. (209). For the reasons presented in § III.H.2, $\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})$ is unbounded. In the expression for $\Sigma^{(1)}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ corresponding to $v\equiv v_c$ in $d=3$ we encounter an equally unbounded local contribution, denoted by $\hbar^{-1}\mathcal{T}^{(1)}(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}')$ (see Eq. (278)). Although $\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})$ and $\mathcal{T}^{(1)}(\boldsymbol{r})$ have different functional forms (among others, whereas $\mathcal{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r})$

[139] Owing to $|\varepsilon|\to\infty$, in § III.I.2 we replace $\Theta(\varepsilon)$ by $\Theta(\varepsilon-\mu)$ where μ stands for the 'chemical potential' introduced in Eq. (22).
[140] The *total* GS number density is positive everywhere.

is identically vanishing when $n_\sigma(\boldsymbol{r}) \equiv n_{\bar\sigma}(\boldsymbol{r})$, $\mathcal{T}^{(1)}(\boldsymbol{r})$ is *never* identically vanishing), they are of the same origin and their unboundedness is rooted in the fact that, up to a multiplicative constant, the Coulomb potential v_c, viewed as an operator, and the single-particle kinetic-energy operator τ are each other's inverses (see Eq. (205)). In this Appendix we shall in the main consider regularization of $\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})$, effected through a summation over an infinite number of unbounded contributions pertaining to $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$, with $m \geq 2$; we denote the regularized extension of $\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})$ by $\widetilde{\mathsf{T}}_{\sigma,\bar\sigma}(\boldsymbol{r};z)$ (for our notational conventions see § III.E.2; see specifically the text following Eq. (111)). The regularized extension of $\mathcal{T}^{(1)}(\boldsymbol{r})$, denoted by $\widetilde{\mathsf{T}}^{(1)}(\boldsymbol{r};z)$, is directly deduced from $\widetilde{\mathsf{T}}_{\sigma,\bar\sigma}(\boldsymbol{r};z)$ through the substitution $(n_{\bar\sigma} - n_\sigma) \rightharpoonup n$ that transforms $\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})$ into $\mathcal{T}^{(1)}(\boldsymbol{r})$ (*cf.* Eqs. (209) and (278)).

The functional similarities between $\mathcal{T}^{(1)}(\boldsymbol{r})$ and $\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})$ and our calculation of $\Sigma^{(1)}_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')$ in § IV.C, confirm that the following regularizing series, deduced solely on the basis of the expression for $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$, correctly produces the pertinent unbounded term pertaining to $\Sigma^{(1)}_{\sigma;\infty_3}(\boldsymbol{r},\boldsymbol{r}')$ upon the substitution $(n_{\bar\sigma} - n_\sigma) \rightharpoonup n$:

$$\begin{aligned}\widetilde{\mathsf{T}}_{\sigma,\bar\sigma}(\boldsymbol{r};z) &:= \frac{1}{z}\sum_{m=1}^{\infty}\int \mathrm{d}^3r''\; v_c(\boldsymbol{r}-\boldsymbol{r}'')\big[n_{\bar\sigma}(\boldsymbol{r}'') - n_\sigma(\boldsymbol{r}'')\big] \\ &\qquad\times\big[\frac{1}{z^m}\tau^m(\boldsymbol{r}'')v_c(\boldsymbol{r}-\boldsymbol{r}'')\big] \\ &= \frac{1}{z^2}\int \mathrm{d}^3r''\; v_c(\boldsymbol{r}-\boldsymbol{r}'')\big[n_{\bar\sigma}(\boldsymbol{r}'') - n_\sigma(\boldsymbol{r}'')\big] \\ &\qquad\times\tau(\boldsymbol{r}'')\big(1-\frac{1}{z}\tau(\boldsymbol{r}'')\big)^{-1} v_c(\boldsymbol{r}-\boldsymbol{r}''), \qquad \text{(G1)}\end{aligned}$$

where the second expression on the RHS is obtained through the formal summation of the geometric series in the first expression (see text following Eq. (111)).

In order to determine a finite-order large-$|z|$ AS for $\widetilde{\mathsf{T}}_{\sigma,\bar\sigma}(\boldsymbol{r};z)$, we first employ the following Fourier representation of the Coulomb potential:

$$v_c(\boldsymbol{r}-\boldsymbol{r}'') = \int \frac{\mathrm{d}^3q}{(2\pi)^3}\,\frac{e^2/\epsilon_0}{\|\boldsymbol{q}\|^2}\,\exp(i\boldsymbol{q}\cdot[\boldsymbol{r}-\boldsymbol{r}'']), \qquad \text{(G2)}$$

from which it readily follows that

$$\begin{aligned}&\tau(\boldsymbol{r}'')\big(1-\frac{1}{z}\tau(\boldsymbol{r}'')\big)^{-1} v_c(\boldsymbol{r}-\boldsymbol{r}'') \\ &\qquad = \frac{e^2\hbar^2}{2m_e\epsilon_0}\int \frac{\mathrm{d}^3q}{(2\pi)^3}\,\frac{\exp(i\boldsymbol{q}\cdot[\boldsymbol{r}-\boldsymbol{r}''])}{1-\hbar^2\|\boldsymbol{q}\|^2/[2m_e z]}. \qquad \text{(G3)}\end{aligned}$$

Using the spherical polar coordinates for $\boldsymbol{q}$, with $\boldsymbol{r}-\boldsymbol{r}''$ the polar axis, the integral on the RHS of Eq. (G3) reduces to $(\hbar^2/[\pi m_e])v_c(\boldsymbol{r}-\boldsymbol{r}'')$ times the one-dimensional integral $\int_0^\infty \mathrm{d}q\, q\sin(aq)/(1-\zeta q^2)$, where $a{:=}\|\boldsymbol{r}-\boldsymbol{r}''\|$ and $\zeta{:=}\hbar^2/(2m_e z)$. Making use of the fact that the integrand of this integral is an *even* function of q, so that $\int_0^\infty \mathrm{d}q\,(\dots) = \frac{1}{2}\int_{-\infty}^\infty \mathrm{d}q\,(\dots)$, applying the residue theorem to two integrals that arise from use of $\sin(aq) = \frac{1}{2i}\{\exp(iaq)-\exp(-iaq)\}$ in the latter integral, we readily obtain

$$\begin{aligned}\tau(\boldsymbol{r}'')\big(1-\frac{1}{z}\tau(\boldsymbol{r}'')\big)^{-1} v_c(\boldsymbol{r}-\boldsymbol{r}'') &= -z\,v_c(\boldsymbol{r}-\boldsymbol{r}'') \\ &\times\exp\big(-\sqrt{2m_e}\,(-z)^{1/2}\|\boldsymbol{r}-\boldsymbol{r}''\|/\hbar\big), \quad \text{(G4)}\end{aligned}$$

where $z^{1/2}$ stands for the principal branch of the square-root function, so that

$$(-z)^{1/2} = \mp i z^{1/2},\quad \left\{\begin{array}{c} 0<\arg(z)<\pi, \\ -\pi<\arg(z)<0. \end{array}\right. \qquad \text{(G5)}$$

Substituting the RHS of Eq. (G4) into that of Eq. (G1), transforming the variable of integration (so that $\boldsymbol{r}''$ in the arguments of $n_{\bar\sigma}(\boldsymbol{r}'')$ and $n_\sigma(\boldsymbol{r}'')$ is changed into $\boldsymbol{r}-\boldsymbol{r}''$), followed by employing the Fourier integral representation (*cf.* Eq. (F147))

$$n_\sigma(\boldsymbol{r}) = \int \frac{\mathrm{d}^3q}{(2\pi)^3}\;\bar n_\sigma(\boldsymbol{q})\,\exp(i\boldsymbol{q}\cdot\boldsymbol{r}), \qquad \text{(G6)}$$

the resulting integration with respect to $\boldsymbol{r}''$ is easily carried out in terms of the spherical polar coordinates of $\boldsymbol{r}''$; making use of the standard result (see Abramowitz and Stegun 1972, p. 1028)

$$\int_0^\infty \mathrm{d}x\;\mathrm{e}^{-sx}\,\frac{\sin(\alpha x)}{x} = \tan^{-1}\Big(\frac{\alpha}{s}\Big),\quad \left\{\begin{array}{l} \mathrm{Re}(s)>0, \\ \mathrm{Im}(\alpha)=0, \end{array}\right.$$

we obtain

$$\begin{aligned}\widetilde{\mathsf{T}}_{\sigma,\bar\sigma}(\boldsymbol{r};z) &= \frac{-4\pi}{z}\Big(\frac{e^2}{4\pi\epsilon_0}\Big)^2\int\frac{\mathrm{d}^3q}{(2\pi)^3}\;\frac{\bar n_{\bar\sigma}(\boldsymbol{q})-\bar n_\sigma(\boldsymbol{q})}{\|\boldsymbol{q}\|} \\ &\quad\times\tan^{-1}\Big(\frac{\|\boldsymbol{q}\|}{\sqrt{2m_e}\,(-z)^{1/2}/\hbar}\Big)\,\exp(i\boldsymbol{q}\cdot\boldsymbol{r}), \qquad \text{(G7)}\end{aligned}$$

where $\tan^{-1}(z)$ stands for the principal branch of the inverse of $\tan(z)$.

Since $\tan^{-1}(z) = \sum_{m=0}^\infty (-1)^m z^{2m+1}/(2m+1)$ is uniformly convergent for $|z|\leq 1$, $z^2 \neq -1$, if follows that in cases where $\bar n_{\bar\sigma}(\boldsymbol{q})-\bar n_\sigma(\boldsymbol{q}) \equiv 0$ for $\|\boldsymbol{q}\| > Q$, with Q some *finite* wavenumber, $(-z)^{1/2}\,\widetilde{\mathsf{T}}_{\sigma,\bar\sigma}(\boldsymbol{r};z)$ has a uniformly convergent series in powers of $1/z$ for $|z| > \hbar^2Q^2/[2m_e]$.

In order to obtain an AS for $\widetilde{\mathsf{T}}_{\sigma,\bar\sigma}(\boldsymbol{r};z)$, $|z|\to\infty$, suitable for a general case, we replace $\bar n_{\bar\sigma}(\boldsymbol{q})-\bar n_\sigma(\boldsymbol{q})$ on the RHS of Eq. (G7) by $\int \mathrm{d}^3r\,[n_{\bar\sigma}(\boldsymbol{r})-n_\sigma(\boldsymbol{r})]\exp(-i\boldsymbol{q}\cdot\boldsymbol{r})$ and exchange the order of integrations. Through formally replacing $\tan^{-1}(\dots)$ in this expression by the above-presented series, we obtain a series involving integrals of the form $\int \mathrm{d}^3q\,\|\boldsymbol{q}\|^{2m}\exp(i\boldsymbol{q}\cdot[\boldsymbol{r}-\boldsymbol{r}'])$, which is equal to $(-1)^m(2\pi)^3\,\nabla_{\boldsymbol{r}}^{2m}\delta(\boldsymbol{r}-\boldsymbol{r}')$. Upon exchanging the order of differentiation and integration we obtain the following formal expression:

$$\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z) = \frac{-4\pi\hbar}{\sqrt{2m_e}} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{(-z)^{1/2} z} \times \sum_{m=0}^{\infty} \frac{1}{2m+1} \frac{1}{z^m} \tau^m(\boldsymbol{r}) \big[n_{\bar{\sigma}}(\boldsymbol{r}) - n_{\sigma}(\boldsymbol{r})\big]. \quad \text{(G8)}$$

With $\sum_{m=0}^{\infty} z^m/(2m+1) = z^{-1/2}\tanh^{-1}(z^{1/2})$, for $|z| < 1$, the result in Eq. (G8) can be written as

$$\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z) = \frac{-4\pi\hbar}{\sqrt{2m_e}} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{(-z)^{1/2} z} \times \frac{\tanh^{-1}\big(\tau^{1/2}(\boldsymbol{r})/z^{1/2}\big)}{\tau^{1/2}(\boldsymbol{r})/z^{1/2}} \big[n_{\bar{\sigma}}(\boldsymbol{r}) - n_{\sigma}(\boldsymbol{r})\big], \quad \text{(G9)}$$

which in essence is an abstract representation of the expression in Eq. (G8); the expressions in Eqs. (G7) and (G9) are more general than the formal expression in Eq. (G8), for with M the smallest finite integer for which $\tau^M(\boldsymbol{r})[n_{\bar{\sigma}}(\boldsymbol{r}) - n_{\sigma}(\boldsymbol{r})]$ is non-integrably unbounded for *some* $\boldsymbol{r}$ (see criterion (B) in § II.B), the terms on the RHS of Eq. (G8) corresponding to $m \geq M$ are *not* directly meaningful. The existence of such an M implies that

$$\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z) \sim \frac{-4\pi\hbar}{\sqrt{2m_e}} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{(-z)^{1/2}} \Big(\frac{1}{z} + \dots + \frac{1/[2M-1]}{z^M} \tau^{M-1}(\boldsymbol{r})\Big) \big[n_{\bar{\sigma}}(\boldsymbol{r}) - n_{\sigma}(\boldsymbol{r})\big] \quad \text{(G10)}$$

constitutes the M leading terms in the AS of $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$ for $|z| \to \infty$ which directly can be Fourier transformed, thus yielding the complete M leading terms in the AS pertaining to the Fourier transform with respect to $\boldsymbol{r}$ of $(-z)^{1/2}\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$ in terms of the asymptotic sequence $\{1, 1/z, \dots\}$; the non-integrability of $\tau^M(\boldsymbol{r})[n_{\bar{\sigma}}(\boldsymbol{r}) - n_{\sigma}(\boldsymbol{r})]$ in a neighbourhood of some $\boldsymbol{r}$ implies that the term immediately subsequent to that decaying like $1/|z|^M$ in the large-$|z|$ AS of the Fourier transform of $(-z)^{1/2}\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$, does *not* decay like $1/|z|^{M+1}$, but more slowly (see § II.B). In Appendix K we deduce and present a direct relationship between the behaviour of $\tau(\boldsymbol{r})n_{\sigma}(\boldsymbol{r})$ and that of the local external potential $u(\boldsymbol{r})$, in $d = 3$ (see in particular Eq. (K16)), from which it follows that for $u(\boldsymbol{r})$ diverging as $\boldsymbol{r} \to \boldsymbol{R}_j$, with $\boldsymbol{R}_j$ the position vector of an ionic nucleus, $\tau(\boldsymbol{r})n_{\sigma}(\boldsymbol{r})$ also diverges, like $u(\boldsymbol{r})$, as $\boldsymbol{r}$ approaches $\boldsymbol{R}_j$, $\forall j$. Since the singularity of $v_c(\boldsymbol{r}-\boldsymbol{r}')$ at $\boldsymbol{r} = \boldsymbol{r}'$ is integrable, it follows that provided $n_{\bar{\sigma}}(\boldsymbol{r}) \not\equiv n_{\sigma}(\boldsymbol{r})$, for $u(\boldsymbol{r}) \propto v_c(\boldsymbol{r} - \boldsymbol{R}_j)$ as $\boldsymbol{r} \to \boldsymbol{R}_j$ (*cf.* Eq. (K6)), $\tau(\boldsymbol{r})[n_{\bar{\sigma}}(\boldsymbol{r}) - n_{\sigma}(\boldsymbol{r})]$ is integrably divergent for $\boldsymbol{r} \to \boldsymbol{R}_j$, $\forall j$. Consequently, the term subsequent to that *decaying* like $1/|z|^{3/2}$ in the large-$|z|$ AS of the Fourier transform of $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$ with respect to $\boldsymbol{r}$ (evidently $[n_{\bar{\sigma}}(\boldsymbol{r}) - n_{\sigma}(\boldsymbol{r})]$ is integrable with respect to $\boldsymbol{r}$) is *not* one decaying more slowly than or as slow as $1/|z|^2$, but more quickly (to be explicit, as quickly as $1/|z|^{5/2}$). Since in the present paper we do *not* consider contributions to the large-$|z|$ AS of $\widetilde{\Sigma}_{\sigma}(\boldsymbol{r},\boldsymbol{r}';z)$ decaying like $1/|z|^m$, with $m > 2$, we conclude that from the perspective of our considerations in this paper, the following asymptotic expression, which can be directly Fourier transformed, is complete (*cf.* Eq. (112))

$$\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z) \sim \frac{\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}|z)}{z^2}, \quad |z| \to \infty, \quad \text{(G11)}$$

where (*cf.* Eq. (110))

$$\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}|z) = \mathsf{T}^{\mathrm{r}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}) + \mathsf{T}^{\mathrm{s_b}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}) + \widetilde{\mathsf{T}}^{\mathrm{s}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}\|z), \quad \text{(G12)}$$

in which (see footnote 31)

$$\mathsf{T}^{\mathrm{r}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}) \equiv 0, \quad \text{(G13)}$$

$$\mathsf{T}^{\mathrm{s_b}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}) \equiv 0, \quad \text{(G14)}$$

$$\widetilde{\mathsf{T}}^{\mathrm{s}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}\|z) \equiv \frac{4\pi\hbar}{\sqrt{2m_e}} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 (-z)^{1/2} \times \big[n_{\bar{\sigma}}(\boldsymbol{r}) - n_{\sigma}(\boldsymbol{r})\big]. \quad \text{(G15)}$$

We have introduced these auxiliary functions in order to conform with the notational convention adopted in this paper (see § III.E.2).

As is apparent from Eq. (G15), $\widetilde{\mathsf{T}}^{\mathrm{s}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}\|z)$ (and thus $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}|z)$) approaches a *purely real* value for $\arg(z) \to \pm\pi$, while it approaches a *purely imaginary* value for $\arg(z) \to 0$ (*cf.* Eq. (G17) below). These observations can be clarified by considering the fact that $\tau(\boldsymbol{r})$ is a positive-definite operator, so that for a real and negative ε, $\big(1 - \tau(\boldsymbol{r})/\varepsilon\big)$ does *not* vanish and consequently, for $z = \varepsilon \pm i\eta$, with $\eta \downarrow 0$, the integral on the RHS of Eq. (G1) *cannot* give rise to an imaginary contribution; for a real and positive ε, on the other hand, $\big(1 - \tau(\boldsymbol{r})/\varepsilon\big)$ does vanish (the spectrum of $\tau(\boldsymbol{r})$ is unbounded from above), thus in this case giving rise to a $\widetilde{\mathsf{T}}^{\mathrm{s}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}\|z)$, and thus a $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}|z)$, that involves an imaginary contribution for $z = \varepsilon \pm i\eta$, $\eta \downarrow 0$.

Following Eq. (G7) above, we have indicated that, in cases where $\bar{n}_{\sigma'}(\boldsymbol{q}) \equiv 0$ for $\|\boldsymbol{q}\| > Q$, with $\sigma' \in \{\sigma, \bar{\sigma}\}$, $n_{\sigma'}(\boldsymbol{r})$ is differentiable with respect to $\boldsymbol{r}$ to any arbitrary finite order so that, for number densities of this type, $(-z)^{1/2}\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z)$ can be described in terms of a uniformly convergent series in powers of $1/z$ for $|z| > \hbar^2 Q^2/[2m_e]$. In the most idealized case of uniform GSs, corresponding to $\bar{n}_{\sigma'}(\boldsymbol{q}) = (2\pi)^3 n_{0;\sigma'}\,\delta(\boldsymbol{q})$, we have

$$\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma}}(\boldsymbol{r};z) \equiv \frac{\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}|z)}{z^2} = \frac{4\pi\hbar}{\sqrt{2m_e}} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 (-z)^{1/2} \frac{n_{0;\bar{\sigma}} - n_{0;\sigma}}{z^2}, \quad \text{(G16)}$$

which in the case of spin-1/2 fermions, is identically vanishing in the paramagnetic phase. With reference to

Eq. (65), for $z = \varepsilon \pm i\eta$, $\eta \downarrow 0$, as $\varepsilon \gtrless \mu$, from Eq. (G16) we readily obtain [141]

$$\mathsf{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r};\varepsilon) = \frac{4\pi\hbar}{\sqrt{2m_e}} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 [n_{0;\bar{\sigma}} - n_{0;\sigma}] \times \frac{\Theta(\mu-\varepsilon) - i\Theta(\varepsilon-\mu)}{|\varepsilon|^{3/2}}. \quad \text{(G17)}$$

In view of our considerations in § III.E.4, we mention that the double Fourier transform of $\widetilde{\mathsf{T}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{r}|z)\,\delta(\boldsymbol{r}-\boldsymbol{r}')$ (see Eq. (H12)), which we denote by $\overline{\overline{\widetilde{\mathsf{T}}}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{q},\boldsymbol{q}'|z)$, has the following form in the case of uniform GSs:

$$\overline{\overline{\widetilde{\mathsf{T}}}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{q},\boldsymbol{q}'|z) = \frac{4\pi\hbar}{\sqrt{2m_e}} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 (-z)^{1/2} \times \big[n_{0;\bar{\sigma}} - n_{0;\sigma}\big]\,\delta_{\boldsymbol{q},\boldsymbol{q}'}. \quad \text{(G18)}$$

Making use of the conventions in § III.E.2, for (see footnote 83)

$$\overline{\overline{\widetilde{\bar{\mathsf{T}}}}}_{\sigma,\bar{\sigma};\infty_2}(\bar{\boldsymbol{q}},\bar{\boldsymbol{q}}'|\bar{z}) := \frac{1}{e_0^3}\,\overline{\overline{\widetilde{\mathsf{T}}}}_{\sigma,\bar{\sigma};\infty_2}(\boldsymbol{q},\boldsymbol{q}'|z) \quad \text{(G19)}$$

we therefore have

$$\overline{\overline{\widetilde{\bar{\mathsf{T}}}}}_{\sigma,\bar{\sigma};\infty_2}(\bar{\boldsymbol{q}},\bar{\boldsymbol{q}}'|\bar{z}) = \frac{3}{\sqrt{2}}\, r_s^2\,(-\bar{z})^{1/2} \times \big[n_{0;\bar{\sigma}}/n_0 - n_{0;\sigma}/n_0\big]\,\delta_{\bar{\boldsymbol{q}},\bar{\boldsymbol{q}}'}. \quad \text{(G20)}$$

We employ this result in § III.E.3, 4 (see Eqs. (114) and (129)). □

APPENDIX H: REGULARIZATION OF THE MOMENTUM REPRESENTATION OF $\Sigma_{\sigma;\infty_2}^{\mathrm{s_b}}$ AND THE DOUBLE FOURIER TRANSFORM OF $\widetilde{\Sigma}_{\sigma;\infty_2}^{\mathrm{s_b}}(\boldsymbol{r},\boldsymbol{r}';z)$

The term $-\hbar^{-1}v^3(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$ as contributing to $\Sigma_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}')$ (see Eqs. (199) and (212)), although perfectly well defined, is in the case where $v \equiv v_c$ in $d=3$ non-integrable (see criterion (B) in § II.B) with respect to either $\boldsymbol{r}$ or $\boldsymbol{r}'$ so that, for instance, it does *not* possess a Fourier representation. With reference to the expressions for $\Sigma_{\sigma;\infty_m}(\boldsymbol{r},\boldsymbol{r}')$ corresponding to $m=0$ and $m=1$ in Eqs. (173) and (185) respectively, we observe that $-\hbar^{-1}v_c^3(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$ is the third term (and the first non-integrable term with respect to $\boldsymbol{r}'$ in a neighbourhood of $\boldsymbol{r}$) in the formal geometric series of the following function:

$$\widetilde{\mathsf{S}}_\sigma(\boldsymbol{r},\boldsymbol{r}';z) := \frac{-1}{\hbar}\,\frac{v_c(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})}{1 - v_c(\boldsymbol{r}-\boldsymbol{r}')/z}. \quad \text{(H1)}$$

In § II.B we discuss in some detail the fact that non-integrable contributions of the type $-\hbar^{-1}v_c^3(\boldsymbol{r}-\boldsymbol{r}')\,\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$ in the AS of $\widetilde{\Sigma}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ for $|z|\to\infty$ do *not* invalidate this as being an AS; however, such series *cannot* be directly used in order to obtain a large-$|z|$ AS pertaining to the momentum representation of the SE *operator* $\widetilde{\Sigma}_\sigma(z)$. In the particular case at hand, the latter series is to be deduced by first determining the double Fourier transform of $\widetilde{\mathsf{S}}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ or a related function. These are the tasks that we undertake to perform in this Appendix.

With reference to our notational convention that we have introduced in § III.E.2, and in view of the fact that the first two terms in the geometric series expansion of $\widetilde{\mathsf{S}}_\sigma(\boldsymbol{r},\boldsymbol{r}';z)$ in Eq. (H1) are integrable functions contributing to $\Sigma_{\sigma;\infty_0}(\boldsymbol{r},\boldsymbol{r}')$ and $\Sigma_{\sigma;\infty_1}(\boldsymbol{r},\boldsymbol{r}')/z$ respectively (see Eqs. (174) and (185)), we have (see text following Eq. (111))

$$\hbar\widetilde{\Sigma}_{\sigma;\infty_2}^{\mathrm{s_b}}(\boldsymbol{r},\boldsymbol{r}';z) \equiv -\frac{1}{z^2}\,\frac{v_c^3(\boldsymbol{r}-\boldsymbol{r}')\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})}{1 - v_c(\boldsymbol{r}-\boldsymbol{r}')/z}, \quad \text{(H2)}$$

which is evidently integrable with respect to $\boldsymbol{r}'$ in any finite neighbourhood of $\boldsymbol{r}'=\boldsymbol{r}$ (see criterion (B) in § II.B). It is readily verified that the RHS of Eq. (H2) also satisfies criterion (C) in § II.B.

Below we evaluate the first two leading terms in the large-$|z|$ AS of the double Fourier transform of $\hbar\widetilde{\Sigma}_{\sigma;\infty_2}^{\mathrm{s_b}}(\boldsymbol{r},\boldsymbol{r}';z)$ with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$. These are the only terms of direct relevance to our considerations in this paper; in particular the expressions for these terms specialized to uniform and isotropic GSs are of direct use in § III.E.

In view of the specific form of the function on the RHS of Eq. (H2), it is convenient to introduce the 'relative' and 'centre of mass' coordinates

$$\boldsymbol{\rho} \equiv \boldsymbol{r}-\boldsymbol{r}', \quad \boldsymbol{\zeta} \equiv \frac{1}{2}(\boldsymbol{r}+\boldsymbol{r}') \quad \text{(H3)}$$

and define (the 'Wigner-transformed' functions)

$$\underaccent{\tilde}{\varrho}_\sigma(\boldsymbol{\zeta},\boldsymbol{\rho}) := \varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}), \quad \text{(H4)}$$

$$\underaccent{\tilde}{\widetilde{\Sigma}}_{\sigma;\infty_2}^{\mathrm{s_b}}(\boldsymbol{\rho},\boldsymbol{\zeta};z) := \widetilde{\Sigma}_{\sigma;\infty_2}^{\mathrm{s_b}}(\boldsymbol{r},\boldsymbol{r}';z). \quad \text{(H5)}$$

With

$$\overline{\underaccent{\tilde}{\varrho}}_\sigma(\boldsymbol{\zeta};\boldsymbol{q}) := \int \mathrm{d}^3\rho\; \underaccent{\tilde}{\varrho}_\sigma(\boldsymbol{\zeta},\boldsymbol{\rho})\,\mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{\rho}}, \quad \text{(H6)}$$

we obtain

$$\hbar\overline{\underaccent{\tilde}{\widetilde{\Sigma}}}_{\sigma;\infty_2}^{\mathrm{s_b}}(\boldsymbol{q};\boldsymbol{\zeta};z) := \int \mathrm{d}^3\rho\; \hbar\underaccent{\tilde}{\widetilde{\Sigma}}_\sigma^{\mathrm{s_b}}(\boldsymbol{\rho},\boldsymbol{\zeta}|z)\,\mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{\rho}}$$
$$= \frac{-1}{z^2}\int \frac{\mathrm{d}^3q'}{(2\pi)^3}\,\overline{\underaccent{\tilde}{\varrho}}_\sigma(\boldsymbol{\zeta};\boldsymbol{q}')\int \mathrm{d}^3\rho\;\frac{v_c^3(\boldsymbol{\rho})}{1 - v_c(\boldsymbol{\rho})/z}\,\mathrm{e}^{-i(\boldsymbol{q}-\boldsymbol{q}')\cdot\boldsymbol{\rho}}$$

[141] The result in this equation (as well as that in Eq. (G16)) is *exact* for *all* ε; however, unless $|\varepsilon|\to\infty$, *no* physical significance can be ascribed to function $\mathsf{T}_{\sigma,\bar{\sigma}}(\boldsymbol{r};\varepsilon)$ nor to its divergence at $\varepsilon = 0$.

$$= \frac{-4\pi}{z^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 \int \frac{\mathrm{d}^3 q'}{(2\pi)^3}\, \frac{\overline{\varrho}_\sigma(\boldsymbol{\zeta};\boldsymbol{q}')}{\|\boldsymbol{q}-\boldsymbol{q}'\|}\, \tilde{g}(\|\boldsymbol{q}-\boldsymbol{q}'\|,\infty;z), \tag{H7}$$

where $\tilde{g}(\|\boldsymbol{q}-\boldsymbol{q}'\|,\infty;z) \equiv \lim_{R\to\infty} \tilde{g}(\|\boldsymbol{q}-\boldsymbol{q}'\|,R;z)$, with $\tilde{g}(\|\boldsymbol{q}\|,R;z)$ defined in Eq. (F149). Following the same procedure as in Appendix F (see § F.5.b), we obtain (*cf.* Eq. (F153))

$$\tilde{g}(q,\infty;z) \sim -q\Big\{(\gamma-1) + \ln\Big(\frac{e^2 q}{4\pi\epsilon_0\varepsilon_0}\Big) - \ln\Big(\frac{-z}{\varepsilon_0}\Big)\Big\}, \quad |z|\to\infty, \tag{H8}$$

where ε_0 is an arbitrary positive constant energy which replaces the e_R in Appendix F. From Eqs. (H7) and (H8) we finally obtain

$$\hbar\widetilde{\overline{\Sigma}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q};\boldsymbol{\zeta};z) \sim -4\pi\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 \times\Big\{\varrho_\sigma(\boldsymbol{\zeta},\boldsymbol{\rho}=\boldsymbol{0})\,\frac{\ln\big(-z/\varepsilon_0\big)}{z^2} -\Big[(\gamma-1)\,\varrho_\sigma(\boldsymbol{\zeta},\boldsymbol{\rho}=\boldsymbol{0}) + \int \frac{\mathrm{d}^3 q'}{(2\pi)^3}\,\overline{\varrho}_\sigma(\boldsymbol{\zeta};\boldsymbol{q}') \times\ln\Big(\frac{\|\boldsymbol{q}-\boldsymbol{q}'\|e^2}{4\pi\epsilon_0\,\varepsilon_0}\Big)\Big]\frac{1}{z^2}\Big\},\quad |z|\to\infty. \tag{H9}$$

We point out that in the case of *non*-uniform GSs, $\varrho_\sigma(\boldsymbol{\zeta},\boldsymbol{\rho}=\boldsymbol{0}) \not\equiv n_\sigma(\boldsymbol{r})$; however, in the case of systems with uniform and isotropic GSs for which $\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$ is a function of $\|\boldsymbol{r}-\boldsymbol{r}'\|$,

$$\varrho_\sigma(\boldsymbol{\zeta},\boldsymbol{\rho}=\boldsymbol{0}) \equiv n_{0;\sigma}. \tag{H10}$$

From this result and Eq. (H9), making use of Eq. (H17) to be presented below, we arrive at the following *exact* leading-order contribution for homogeneous systems of fermions with uniform and isotropic GSs:

$$\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}';z) \sim -\frac{4\pi}{\hbar}\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 n_{0;\sigma}\,\frac{\ln\big(-z/\varepsilon_0\big)}{z^2}\,\delta_{\boldsymbol{q},\boldsymbol{q}'}, \quad |z|\to\infty. \tag{H11}$$

We point out that, according to our conventions introduced in § III.E.2, the RHS of Eq. (H11) is simply the leading contribution to $\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}'\|z)/z^2$ (see footnote 72); with reference to our convention in this paper (see footnote 31), we note that $\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}'\|z)$ *can* involve a z-independent contribution, which from Eq. (H9) can be seen to be indeed the case for the $\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}'\|z)$ considered here (see Eq. (H18) below). When appropriate, we denote the z-independent contribution to $\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}'\|z)$ by $\overline{\overline{\Sigma}}{}^{\mathrm{s_b}}_{\sigma;\infty_m}(\boldsymbol{q},\boldsymbol{q}')$ (see Eq. (113) and footnote 72).

For completeness we note that the double Fourier transform [142]

$$\overline{\overline{f}}(\boldsymbol{q},\boldsymbol{q}') {:=} \frac{1}{\Omega}\int \mathrm{d}^3 r\mathrm{d}^3 r'\; \mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\, f(\boldsymbol{r},\boldsymbol{r}')\,\mathrm{e}^{i\boldsymbol{q}'\cdot\boldsymbol{r}'} \tag{H12}$$

can be expressed in terms of

$$\underline{f}(\boldsymbol{\rho},\boldsymbol{\zeta}) {:=} f(\boldsymbol{r},\boldsymbol{r}') \tag{H13}$$

as follows

$$\overline{\overline{f}}(\boldsymbol{q},\boldsymbol{q}') = \frac{1}{\Omega}\int \mathrm{d}^3\rho\,\mathrm{d}^3\zeta\;\mathrm{e}^{-i(\boldsymbol{q}+\boldsymbol{q}')\cdot\boldsymbol{\rho}/2}\,\underline{f}(\boldsymbol{\rho},\boldsymbol{\zeta})\,\mathrm{e}^{i(\boldsymbol{q}'-\boldsymbol{q})\cdot\boldsymbol{\zeta}}. \tag{H14}$$

Thus with

$$\boldsymbol{Q} {:=} \frac{1}{2}(\boldsymbol{q}'+\boldsymbol{q}),\quad \boldsymbol{Z} {:=} \boldsymbol{q}'-\boldsymbol{q}, \tag{H15}$$

we have

$$\overline{\overline{f}}(\boldsymbol{q},\boldsymbol{q}') \equiv \overline{\overline{\underline{f}}}(\boldsymbol{Q},\boldsymbol{Z}). \tag{H16}$$

Making use of this result, the double Fourier transform of $\widetilde{\Sigma}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}';z)$ is obtained from

$$\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}';z) \equiv \frac{1}{\Omega}\int \mathrm{d}^3\zeta\,\widetilde{\overline{\Sigma}}{}^{\mathrm{s_b}}_{\sigma}\big((\boldsymbol{q}+\boldsymbol{q}')/2;\boldsymbol{\zeta};z\big)\,\mathrm{e}^{i(\boldsymbol{q}'-\boldsymbol{q})\cdot\boldsymbol{\zeta}}. \tag{H17}$$

We point out that, in the case of uniform and isotropic GSs, $\widetilde{\overline{\Sigma}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q};\boldsymbol{\zeta};z)$ is *independent* of $\boldsymbol{\zeta}$ (see Eq. (H3) above); with reference to Eq. (H10), the RHS of Eq. (H9) is readily verified to obey this expected behaviour. The independence with respect to $\boldsymbol{\zeta}$ of $\widetilde{\overline{\Sigma}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q};\boldsymbol{\zeta};z)$ in the case of uniform and isotropic GSs implies that $\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}';z)$ is equal to $\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q};\boldsymbol{\zeta};z)$ times $(2\pi)^3\delta(\boldsymbol{q}-\boldsymbol{q}')/\Omega \equiv \delta_{\boldsymbol{q},\boldsymbol{q}'}$; from this, making use of Eqs. (H9) and (H10), we readily obtain (*cf.* Eq. (H11) above)

$$\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}';z) \sim -\frac{4\pi}{\hbar}\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 n_0\,\Big\{\frac{n_{0;\sigma}}{n_0}\,\frac{\ln(-z/\varepsilon_0)}{z^2} -\Big[(\gamma-1)\frac{n_{0;\sigma}}{n_0} + \int\frac{\mathrm{d}^3 q''}{(2\pi)^3}\,\frac{\overline{\varrho}{}^{\mathrm{h}}_\sigma(\|\boldsymbol{q}''\|)}{n_0} \times\ln\Big(\frac{e^2\|\boldsymbol{q}-\boldsymbol{q}''\|}{4\pi\epsilon_0\varepsilon_0}\Big)\Big]\frac{1}{z^2}\Big\}\,\delta_{\boldsymbol{q},\boldsymbol{q}'},\quad |z|\to\infty. \tag{H18}$$

Considering spin-1/2 fermions in the paramagnetic phase, replacing $\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$ in Eq. (H2) by its Slater-Fock

[142] Our convention, involving $1/\Omega$, implies use of box boundary condition.

counterpart as presented in Eq. (F24), we obtain the following expression within the framework of the SSDA (*cf.* Eq. (H18) above) [143]

$$\left.\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}';z)\right|_{\mathrm{s}} \sim -\frac{4\pi}{\hbar}\,\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 n_0\,\Big\{\frac{1}{2}\,\frac{\ln\big(-z/\varepsilon_0\big)}{z^2}$$
$$+\Big(\frac{1}{32}\,\frac{k_F}{\|\boldsymbol{q}\|}\Big[(1-\|\boldsymbol{q}\|/k_F)^3(3+\|\boldsymbol{q}\|/k_F)\ln\big(\frac{e^2|k_F-\|\boldsymbol{q}\||}{4\pi\epsilon_0\varepsilon_0}\big)$$
$$-(1+\|\boldsymbol{q}\|/k_F)^3(3-\|\boldsymbol{q}\|/k_F)\ln\big(\frac{e^2|k_F+\|\boldsymbol{q}\||}{4\pi\epsilon_0\varepsilon_0}\big)\Big]$$
$$-\big[(\|\boldsymbol{q}\|/k_F)^2/16+\gamma/2-41/48\big]\Big)\frac{1}{z^2}\Big\}\,\delta_{\boldsymbol{q},\boldsymbol{q}'},\quad |z|\to\infty, \tag{H19}$$

where ε_0 stands for an arbitrary positive constant energy. In deducing this result, we have employed $n_{0;\sigma} = k_F^3/[6\pi^2]$ for the partial number density of the spin-1/2 fermions in the paramagnetic state.

In the calculations of § III.I, we require the imaginary part of the RHS of Eq. (H18) for $z = \varepsilon \pm i\eta$, $\eta \downarrow 0$, as $\varepsilon \to \pm\infty$; with reference to the definition in Eq. (65), from Eq. (H18) for $|\varepsilon| \to \infty$ we readily obtain

$$\mathrm{Re}[\overline{\overline{\Sigma}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}';\varepsilon)] \sim \frac{-4\pi}{\hbar}\,\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 n_{0;\sigma}\,\frac{\ln(|\varepsilon|/\varepsilon_0)}{\varepsilon^2}\,\delta_{\boldsymbol{q},\boldsymbol{q}'}, \tag{H20}$$

$$\mathrm{Im}[\overline{\overline{\Sigma}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}';\varepsilon)] \sim \frac{4\pi^2}{\hbar}\,\left(\frac{e^2}{4\pi\epsilon_0}\right)^3 n_{0;\sigma}\,\frac{\Theta(\varepsilon)}{\varepsilon^2}\,\delta_{\boldsymbol{q},\boldsymbol{q}'}. \tag{H21}$$

It is important to point out that the apparent dependence on ε_0 of $\mathrm{Re}[\overline{\overline{\Sigma}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}';\varepsilon)]$ in Eq. (H20) is a consequence of *not* presenting the next-to-leading-order term in the AS for this function; making use of $(1-\|\boldsymbol{q}\|/k_F)^3(3+\|\boldsymbol{q}\|/k_F) - (1+\|\boldsymbol{q}\|/k_F)^3(3-\|\boldsymbol{q}\|/k_F) = -16\,\|\boldsymbol{q}\|/k_F$, as well as $n_{0;\sigma} = k_F^3/[6\pi^2]$ (for uniform and isotropic systems of spin-1/2 fermions in the paramagnetic GS), from the expression on the RHS of Eq. (H19) we readily deduce that (at least) the *value* of $\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}';z)|_{\mathrm{s}}$ in Eq. (H19) does *not* depend on the *value* of ε_0.

Following the conventions in § III.E.1, replacing ε_0 by e_0 as defined in Eq. (103), for (*cf.* Eq. (104) and see the subsequent text)

$$\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\bar{\boldsymbol{q}},\bar{\boldsymbol{q}}';\bar{z}) := \frac{1}{e_0}\,\hbar\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{q},\boldsymbol{q}';z) \tag{H22}$$

we obtain (for systems of spin-1/2 fermions)

$$\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\bar{\boldsymbol{q}},\bar{\boldsymbol{q}}';\bar{z}) \sim -3\,r_s^3\,\Big\{\frac{1}{2}\,\frac{\ln(-\bar{z})}{\bar{z}^2} - \frac{1}{2}\,\frac{\ln(r_s)}{\bar{z}^2}$$
$$-\Big[\frac{1}{2}(\gamma-1) + \int \frac{\mathrm{d}^3q''}{(2\pi)^3}\,\frac{\overline{\varrho}{}^{\mathrm{h}}_{\sigma}(\|\boldsymbol{q}''\|)}{n_0}$$
$$\times\ln\big(\|\bar{\boldsymbol{q}}-r_0\boldsymbol{q}''\|\big)\Big]\frac{1}{\bar{z}^2}\Big\}\,\delta_{\bar{\boldsymbol{q}},\bar{\boldsymbol{q}}'},\quad |\bar{z}|\to\infty, \tag{H23}$$

where r_0 stands for average distance between the particles (independent of their spin indices) in the GS defined in Eq. (93). Similarly,

$$\left.\widetilde{\overline{\overline{\Sigma}}}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\bar{\boldsymbol{q}},\bar{\boldsymbol{q}}';\bar{z})\right|_{\mathrm{s}} \sim -3\,r_s^3\,\Big\{\frac{1}{2}\,\frac{\ln(-\bar{z})}{\bar{z}^2} - \frac{1}{2}\,\frac{\ln(r_s)}{\bar{z}^2}$$
$$+\Big(\frac{1}{32}\,\frac{\bar{k}_F}{\|\bar{\boldsymbol{q}}\|}\Big[(1-\|\bar{\boldsymbol{q}}\|/\bar{k}_F)^3(3+\|\bar{\boldsymbol{q}}\|/\bar{k}_F)\ln(|\bar{k}_F-\|\bar{\boldsymbol{q}}\||)$$
$$-(1+\|\bar{\boldsymbol{q}}\|/\bar{k}_F)^3(3-\|\bar{\boldsymbol{q}}\|/\bar{k}_F)\ln(|\bar{k}_F+\|\bar{\boldsymbol{q}}\||)\Big]$$
$$-\big[(\|\bar{\boldsymbol{q}}\|/\bar{k}_F)^2/16+\gamma/2-41/48\big]\Big)\frac{1}{\bar{z}^2}\Big\}\,\delta_{\bar{\boldsymbol{q}},\bar{\boldsymbol{q}}'},\quad |\bar{z}|\to\infty. \tag{H24}$$

For completeness, for $d = 3$ and for spin-1/2 fermions in the paramagnetic phase we have $\bar{k}_F = (9\pi/4)^{1/3}$. Note the equality of the first two contributions on the RHS of Eq. (H23) with those on the RHS of Eq. (H24). Above we have indicated that the equality of the first contributions on the RHSs of Eqs. (H23) and (H24) is a direct consequence of the relationship in Eq. (H10). Since, for $r_s \to 0$, $\overline{\varrho}{}^{\mathrm{h}}_{\sigma}(\|\boldsymbol{q}''\|) \to \overline{\varrho}{}^{\mathrm{h}}_{\mathrm{s};\sigma}(\|\boldsymbol{q}''\|)$, it follows that, as $r_s \to 0$, the $\boldsymbol{q}''$ integral on the RHS of Eq. (H23) *cannot* be capable of producing a contribution proportional to $\ln(r_s)$ (although it may produce a result proportional to $r_s\ln(r_s)$), so that the equality of the second contributions on the RHSs of Eqs. (H23) and (H24) *is* exact, independent of the value of r_s. □

[143] In evaluating the expression in Eq. (H19) directly from Eq. (H18), one encounters integrals that turn out to be extremely unwieldy (with the exception of the case corresponding to $\boldsymbol{q} = \boldsymbol{0}$). We have obtained the result in Eq. (H19) by determining the asymptotic terms *after* evaluation of the Fourier transform of $\widetilde{\Sigma}{}^{\mathrm{s_b}}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}';z)$ as presented in Eq. (H2). Although this approach gives rise to somewhat lengthy algebra, nonetheless the technique on which our derivations in Appendix F.5.b is based made it possible to bypass evaluation of integrals that are at least very difficult to express in closed form.

APPENDIX I: TWO BASIC INTEGRALS

In this work we encounter two integrals of the forms

$$\left.\begin{aligned}\mathcal{I}_1(\zeta';\alpha) &:= \int_{\zeta'}^{\infty}\mathrm{d}z\,\frac{\exp(i\alpha z)}{z}\\ \mathcal{I}_2(\zeta';\alpha) &:= \int_{\zeta'}^{\infty}\mathrm{d}z\,\frac{\exp(-i\alpha z)}{z}\end{aligned}\right\}\quad \alpha > 0, \tag{I1}$$

where ζ' is a complex variable. These integrals which enter into our calculations through, for instance, the following expression

$$\int_0^\infty \mathrm{d}x\, \frac{\sin(\alpha x)}{x+\zeta'} \equiv \int_{\zeta'}^\infty \mathrm{d}z\, \frac{\sin(\alpha[z-\zeta'])}{z}$$
$$= \frac{1}{2i}\big\{ \mathrm{e}^{-i\alpha\zeta'}\, \mathcal{I}_1(\zeta';\alpha) - \mathrm{e}^{i\alpha\zeta'}\, \mathcal{I}_2(\zeta';\alpha)\big\}, \qquad \text{(I2)}$$

can be expressed in terms of the exponential-integral function (Gradshtyn and Ryzhik 1965, p. 925)

$$\mathrm{Ei}(z) := -\int_{-z}^\infty \mathrm{d}\zeta\, \frac{\exp(-\zeta)}{\zeta}; \qquad \text{(I3)}$$

the contour of integration in the complex ζ plane is depicted in Fig. 1 (for some related considerations see Sansone and Gerretsen (1960, pp. 406-412)). This function has two branch points: one at $z=0$ and the other at $1/z=0$. The principal branch of $\mathrm{Ei}(z)$, with $\arg(-z)\in(-\pi,\pi)$, is specified by the requirement that $\mathrm{Ei}(x)$ be real for $x<0$. In the present work we employ *truncated* forms of the following series (Gradshtyn and Ryzhik 1965, p. 927):

$$\mathrm{Ei}(z) = \gamma + \ln(-z) + \sum_{k=1}^\infty \frac{z^k}{k\,k!}, \qquad \text{(I4)}$$

in the asymptotic regime $|z|\to 0$; in our consideration we need to employ AS of up to and including $z^5/600$. Here $\gamma = 0.577\ 215\ 66\ldots$ stands for the Euler constant and ln for the principal branch of the logarithm function for which we have $\ln(-z) = \ln|z| + i\arg(-z)$, with $\arg(-z)\in(-\pi,\pi)$. For clarity, the imaginary part of the 'principal branch' of the logarithm function is equal to the 'arg' (or 'phase') of its argument as measured with respect to the positive real axis, with 'arg' covering the range $(-\pi,\pi)$; the requirement concerning measurement of the 'arg' with respect to the positive real axis is *not* affected by the location of the branch cut in the z plane of the functions under consideration; thus $\arg(-z)$ is similar to $\arg(z)$ measured with respect to the positive real axis (see Fig. 1), even though the branch cut of $\ln(-z)$ is located along the positive real axis, to be contrasted with that of $\ln(z)$ which is along the negative real axis. Note in passing that $\ln(-z) = \ln(z) \mp i\pi$, $\arg(z) \gtrless 0$.

In dealing with $\mathcal{I}_1(\zeta';\alpha)$ and $\mathcal{I}_2(\zeta';\alpha)$, careful account has to be taken of the multi-valued nature of $\mathrm{Ei}(z)$. To appreciate the significance of this, consider

$$\mathcal{J}_C(z) := \int_C \mathrm{d}\zeta\, \frac{\exp(-\zeta)}{\zeta}, \qquad \text{(I5)}$$

where the integration is carried out along the contour C as depicted in Fig. 2. As can be seen from this Figure, $\mathcal{J}_C(z)$ can be expressed in terms of $\mathrm{Ei}(z)$, provided that C is supplemented by the contour δ^+, depicted as a broken line. By the Cauchy theorem we have

$$\mathcal{J}_C(z) = -2\pi i - \mathrm{Ei}(z) \equiv -2\pi i + \mathcal{J}_{C'}(z); \qquad \text{(I6)}$$

the difference $-2\pi i$ between $\mathcal{J}_C(z)$ and $-\mathrm{Ei}(z)$ is attributable to the branch-cut discontinuity of $\ln(-z)$ in the expression on the RHS of Eq. (I4) for $-z$ along the negative real axis.

In order to express $\mathcal{I}_1(\zeta';\alpha)$ in terms of Ei, we first apply the variable transformation $-i\alpha z \rightharpoonup z$, upon which (since we have assumed $\alpha>0$) ζ' is rotated *clockwise* by $\pi/2$ around the origin while its distance from the origin is multiplied by α. Since ζ' is an end-point of the contour of integration, the transformation $-i\alpha z \rightharpoonup z$ "drags along" the contour in the manner shown in Figs. 3 and 4. As can be directly seen from Fig. 4, in the case where $\arg(\zeta')\in(-\pi,-\pi/2)$, the transformation $-i\alpha z\rightharpoonup z$ gives rise to ζ' crossing the negative real axis in its change to $-i\alpha\zeta'$. In a manner similar to the treatment of $\mathcal{J}_C(z)$ presented above, we obtain

$$\mathcal{I}_1(\zeta';\alpha) = \begin{cases} -\mathrm{Ei}(i\alpha\zeta'), & \arg(\zeta')\in(-\pi/2,\pi) \\[2ex] -\mathrm{Ei}(i\alpha\zeta') + 2\pi i, & \arg(\zeta')\in(-\pi,-\pi/2). \end{cases} \qquad \text{(I7)}$$

Along the same lines as presented above, employing, however, the variable transformation $i\alpha z\rightharpoonup z$ which for $\alpha>0$ brings about a *counter-clockwise* rotation by $\pi/2$ of ζ' around the origin together with changing the amplitude of ζ' into $\alpha|\zeta'|$, for $\mathcal{I}_2(\zeta';\alpha)$ we obtain (see Figs. 5 and 6)

$$\mathcal{I}_2(\zeta';\alpha) = \begin{cases} -\mathrm{Ei}(-i\alpha\zeta'), & \arg(\zeta')\in(-\pi,\pi/2) \\[2ex] -\mathrm{Ei}(-i\alpha\zeta') - 2\pi i, & \arg(\zeta')\in(\pi/2,\pi). \end{cases} \qquad \text{(I8)}$$

□

APPENDIX J: ASYMPTOTIC BEHAVIOUR OF THE DENSITY MATRICES PERTAINING TO UNIFORM AND ISOTROPIC FERMI LIQUIDS

In several instances in this paper, knowledge of the behaviour of the single-particle density matrix $\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r})$, pertaining to uniform and isotropic GSs, for $\|\boldsymbol{r}-\boldsymbol{r}'\|\to\infty$ turns out to be of crucial significance. Here we deduce the first two leading terms in the large-r AS of $\varrho_\sigma^{\mathrm{h}}(r)$ for systems in $d=3$ (*cf.* Eq. (F9)), with special emphasis on Fermi-liquid metallic states.

From the definition of the single-particle GF $G_\sigma(\boldsymbol{r}t,\boldsymbol{r}'t')$ in Eq. (E7), it is readily deduced that (see Eq. (B16))

$$\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) = -iG_\sigma(\boldsymbol{r}t,\boldsymbol{r}'t^+), \qquad \text{(J1)}$$

where t^+ is infinitesimally larger than t. Specializing to uniform and isotropic GSs for which $G_\sigma(\boldsymbol{r}t,\boldsymbol{r}'t')$ is a function of $\|\boldsymbol{r}-\boldsymbol{r}'\|$, with

$$\mathsf{n}_\sigma(\boldsymbol{k}) := \langle \Psi_{N;0} | \hat{\mathsf{a}}^\dagger_{\boldsymbol{k};\sigma} \hat{\mathsf{a}}_{\boldsymbol{k};\sigma} | \Psi_{N;0} \rangle \tag{J2}$$

the GS momentum distribution function (*cf.* Eq. (A7)), we have

$$\varrho_\sigma^{\rm h}(\|\boldsymbol{r}-\boldsymbol{r}'\|) = \int \frac{{\rm d}^3 k}{(2\pi)^3}\, {\rm e}^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\, \mathsf{n}_\sigma(\|\boldsymbol{k}\|)$$
$$= \frac{1}{2\pi^2 \|\boldsymbol{r}-\boldsymbol{r}'\|} \int_0^\infty {\rm d}k\; k\, \mathsf{n}_\sigma(k)\, \sin(k\|\boldsymbol{r}-\boldsymbol{r}'\|), \tag{J3}$$

where we have chosen to suppress the subscript 'h' in $\mathsf{n}_\sigma^{\rm h}(k)$ (see Eq. (F9)) that would visibly distinguish this *isotropic* function from its more general counterpart $\mathsf{n}_\sigma(\boldsymbol{k})$; we shall adhere to this choice in the remaining part of this Appendix. For completeness, according to Yasuhara and Kawazoe (1976), for uniform and isotropic electron systems in the paramagnetic phase one has (below $\mathsf{n}(k) := \sum_{\sigma=\uparrow,\downarrow} \mathsf{n}_\sigma(k)$)

$$\mathsf{n}(k) \sim \frac{4 m_e^2}{\pi^2 (9\pi)^{4/3} \hbar^4} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 n_0^{-2/3} \mathsf{g}(0) \left(\frac{k_F}{k}\right)^8, \quad \text{for } k \to \infty, \tag{J4}$$

where $\mathsf{g}(0)$ stands for the normalized total pair correlation function $\mathsf{g}(r)$ at $r=0$ (see Appendix F, § F.1.d, in particular Eq. (F106)); according to Yasuhara (1972), for $\mathsf{g}(0)$ one has the following *approximate* result

$$\mathsf{g}(0) = \frac{1}{8}\left(\frac{x}{I_1(x)}\right)^2, \quad x := \frac{4 m_e^{1/2}}{3^{1/6}\pi^{5/6}\hbar} \left(\frac{e^2}{4\pi\epsilon_0}\right)^{1/2} n_0^{-1/6}, \tag{J5}$$

where $I_1(x)$ stands for the modified Bessel function of first kind and first order (Abramowitz and Stegun 1972, p. 374). The expression on the RHS of Eq. (J4) shows that the upper boundary of the k integral on the RHS of Eq. (J3) can be reduced from ∞ to some finite multiple of $k_{F;\sigma}$ without considerably affecting the behaviour of $\varrho_\sigma^{\rm h}(\|\boldsymbol{r}-\boldsymbol{r}'\|)$; in fact, as we shall see below, the behaviour of the first two leading terms in the AS of this function for $\|\boldsymbol{r}-\boldsymbol{r}'\| \to \infty$ is fully determined by the behaviour of $\mathsf{n}_\sigma(k)$ for k in some infinitesimal neighbourhood of $k_{F;\sigma}$, the Fermi wavenumber pertaining to fermions with spin index σ. We note that, in the paramagnetic phase, $\mathsf{n}(k)$ as calculated within the framework of the random-phase approximation (RPA) also decays like $1/k^8$ as $k \to \infty$ (Daniel and Vosko 1960). On the other hand, this decay is like $1/k^4$ according to the calculations by Belyakov (1961). Although both outcomes concern $d=3$, the result by the former workers corresponds to $v \equiv v_c$, whereas that by the latter researcher corresponds to the extreme limit of a short-range v.

Subdividing (in anticipation of the discontinuity of $\mathsf{n}_\sigma(k)$ at $k = k_{F;\sigma}$) the k integral on the RHS of Eq. (J3) into two, covering the intervals $[0, k_{F;\sigma})$ and $(k_{F;\sigma}, \infty)$, upon twice applying of integration by parts, we obtain [144]

$$\varrho_\sigma^{\rm h}(r) = -\frac{Z_{F;\sigma}\, k_{F;\sigma}}{2\pi^2} \frac{\cos(k_{F;\sigma}\, r)}{r^2} + \frac{1}{2\pi^2}\Big\{ Z_{F;\sigma}$$
$$+ k_{F;\sigma} \Big[\frac{\rm d}{{\rm d}k}\mathsf{n}_\sigma(k)\Big|_{k\uparrow k_{F;\sigma}} - \frac{\rm d}{{\rm d}k}\mathsf{n}_\sigma(k)\Big|_{k\downarrow k_{F;\sigma}} \Big]\Big\} \frac{\sin(k_{F;\sigma}\, r)}{r^3}$$
$$-\frac{1}{2\pi^2 r^3}\, \wp\!\int_0^\infty {\rm d}k\, \Big[\frac{{\rm d}^2}{{\rm d}k^2}\, k\, \mathsf{n}_\sigma(k)\Big] \sin(k\, r), \tag{J6}$$

where the Cauchy principal-value integral excludes an infinitesimal interval centred at $k = k_{F;\sigma}$, and (Migdal 1957, Luttinger 1960)

$$Z_{F;\sigma} := \mathsf{n}_\sigma(k_{F;\sigma} - 0^+) - \mathsf{n}_\sigma(k_{F;\sigma} + 0^+). \tag{J7}$$

Provided that the terms enclosed by square brackets (involving the left and right derivatives of $\mathsf{n}_\sigma(k)$ at $k = k_{F;\sigma}$) as well as the principal-value integral over $[0,\infty)$ exist, the expression in Eq. (J6) is an *exact* reformulation of that in Eq. (J3). [145] When this is the case, by the Riemann-Lebesgue lemma (Whittaker and Watson 1927, p. 172) we have

$$\wp\!\int_0^\infty {\rm d}k\, \Big[\frac{{\rm d}^2}{{\rm d}k^2}\, k\, \mathsf{n}_\sigma(k)\Big] \sin(k\, r) = o(1) \quad \text{for} \quad r \to \infty, \tag{J8}$$

so that by disregarding the k integral on the RHS of Eq. (J6), we retain an AS of $\varrho_\sigma^{\rm h}(r)$ for $r \to \infty$, involving the two most leading terms of the complete AS of this function (see § II.B); compare the first term on the RHS of Eq. (J6) with the RHS of Eq. (F19) and note that the effect of interaction on the leading-order term in the large-r AS for $\varrho_\sigma^{\rm h}(r)$ is reduction of the magnitude of the corresponding non-interacting term by the factor $Z_{F;\sigma}$ (for completeness, compare the leading-order term on the RHS of Eq. (J6) with its counterpart in $d=2$ as derived and presented by Farid (2000a)). From the series in Eq. (J6) it is directly evident that the two leading terms in the large-r AS for $\varrho_\sigma^{\rm h}(r)$ are solely determined by $k_{F;\sigma}$, $\mathsf{n}_\sigma(k_{F;\sigma} - 0^+) - \mathsf{n}_\sigma(k_{F;\sigma} + 0^+)$ and ${\rm d}\mathsf{n}_\sigma(k)/{\rm d}k|_{k\uparrow k_{F;\sigma}} - {\rm d}\mathsf{n}_\sigma(k)/{\rm d}k|_{k\downarrow k_{F;\sigma}}$. Provided that the application of integration by parts to the k integral on the RHS of Eq. (J6) does not lead to any unbounded

[144] In this Appendix we tacitly assume that, with the exception of $k = k_{F;\sigma}$, $\mathsf{n}_\sigma(k)$ is *everywhere* continuous and, unless explicitly specified otherwise, sufficiently many times differentiable.

[145] Thus, for instance, by replacing $\mathsf{n}_\sigma(k)$ in Eq. (J6) by $\mathsf{n}_{{\rm s};\sigma}(k) := \Theta(k_{F;\sigma} - k)$ and identifying $Z_{F;\sigma}$ with unity, we immediately obtain the exact expression for $\varrho_{{\rm s};\sigma}^{\rm h}(r)$ in Eq. (F24). In this connection, note that the left and right derivatives of $\mathsf{n}_{{\rm s};\sigma}(k)$ with respect to k at $k = k_{F;\sigma}$ are identically vanishing.

contribution, [146] it can be directly verified that the third leading term in the large-r AS of $\varrho_\sigma^{\rm h}(r)$ is in addition also partly determined by $\mathsf{d}\mathsf{n}_\sigma(k)/\mathrm{d}k|_{k\downarrow 0}$ which at least in the weak-coupling regime, if non-vanishing, should be rather small (*cf.* Eq. (9) in the paper by Daniel and Vosko (1960)).

Finally, general considerations show (Farid 1999c; see § 6, and in particular the third paragraph) [147] that, in the case of Fermi liquids, it is in principle possible that $\mathsf{d}\mathsf{n}_\sigma(k)/\mathrm{d}k$ is divergent for both $k \uparrow k_{F;\sigma}$ and $k \downarrow k_{F;\sigma}$. Whereas this is not the case according to the RPA for $\mathsf{n}(k)$ as calculated by Daniel and Vosko (1960), the $\mathsf{n}(k)$ due to Belyakov (1961) has the following form in the vicinity of $k = k_F$ (see text following Eq. (A70) in Appendix A)

$$\mathsf{n}(k) \sim \mathsf{n}(k_F \mp 0^+) + \mathsf{A}\,(k/k_F - 1)\ln|k/k_F - 1|, \quad \begin{array}{l} k \uparrow k_F \\ k \downarrow k_F \end{array} \tag{J9}$$

where A stands for a (positive) constant. From this expression, one deduces that

$$\frac{\mathsf{d}\mathsf{n}(k)}{\mathrm{d}k} \sim \frac{\mathsf{A}}{k_F}\,\big\{\ln|k/k_F - 1| + 1\big\}, \quad k \to k_F,$$

and that

$$\frac{\mathrm{d}^2\mathsf{n}(k)}{\mathrm{d}k^2} \sim \frac{\mathsf{A}/k_F}{k - k_F}, \quad k \to k_F,$$

so that not only the (divergent) contributions enclosed by square brackets on the RHS of Eq. (J6) *entirely* cancel, but also the integral on the RHS of Eq. (J6) is bounded. Thus Eq. (J6) indeed also applies to such (unconventional) Fermi-liquid metallic states as that dealt with by Belyakov (1961). □

APPENDIX K: ON THE DIFFERENTIABILITY PROPERTY OF THE GROUND-STATE PARTIAL NUMBER DENSITIES

In § III.H.2, we encounter the *unbounded* function $\mathcal{T}_{\sigma,\bar\sigma}(\boldsymbol{r})$ (see Eq. (209)) whose regularization, with which we deal in Appendix G, results in $\widetilde{\mathsf{T}}_{\sigma,\bar\sigma}(\boldsymbol{r};z)$. The leading asymptotic term of this function for $|z| \to \infty$, namely $\widetilde{\mathsf{T}}^{\rm s}_{\sigma,\bar\sigma;\infty_2}(\boldsymbol{r}\|z)$ (see Eqs. (G1), (G11) and (G15)), [148] contributes to $\widetilde{\Sigma}^{\rm s}_{\sigma;\infty_2}(\boldsymbol{r},\boldsymbol{r}'\|z)$ presented in Eq. (213). In Appendix G we discuss the significance of the value for the smallest integer M for which $\tau^M(\boldsymbol{r})[n_{\bar\sigma}(\boldsymbol{r}) - n_\sigma(\boldsymbol{r})]$ becomes non-integrably unbounded for *some* $\boldsymbol{r}$ (see criterion (B) in § II.B). Here we investigate the differentiability property of the partial number densities $\{n_\sigma(\boldsymbol{r})\}$ with respect to $\boldsymbol{r}$. In doing so, we pay especial attention to the case where the ionic potential $u(\boldsymbol{r})$ is a linear superposition of electrostatic Coulomb potentials (in $d = 3$) centred at the ionic positions $\{\boldsymbol{R}_j\}$. For this case we demonstrate that $\tau(\boldsymbol{r})n_\sigma(\boldsymbol{r}) \sim 2Z_j v_c(\boldsymbol{r} - \boldsymbol{R}_j)n_\sigma(\boldsymbol{R}_j)$ for $\boldsymbol{r} \to \boldsymbol{R}_j$ (see Eqs. (K6) and (K16) below) where $Z_j > 0$ stands for the effective atomic number [149] of the ion at $\boldsymbol{R}_j$; although divergent like $1/\|\boldsymbol{r} - \boldsymbol{R}_j\|$ for $\boldsymbol{r} \to \boldsymbol{R}_j$, $\tau(\boldsymbol{r})n_\sigma(\boldsymbol{r})$ is integrable. Consequently we deduce that the second term in the large-$|z|$ AS for the Fourier transform with respect to $\boldsymbol{r}$ of $\widetilde{\mathsf{T}}_{\sigma,\bar\sigma}(\boldsymbol{r};z)$ decays more rapidly than $1/|z|^2$ (see Eq. (G10)).

Applying $\tau(\boldsymbol{r})$ to both sides of the defining expression for $n_\sigma(\boldsymbol{r})$ (see Eq. (163)),

$$n_\sigma(\boldsymbol{r}) := \langle \Psi_{N;0}|\hat\psi^\dagger_\sigma(\boldsymbol{r})\hat\psi_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle, \tag{K1}$$

while making use of chain rule of differentiation and

$$\begin{aligned}\langle \Psi_{N;0}|\big[\tau(\boldsymbol{r})\hat\psi^\dagger_\sigma(\boldsymbol{r})\big]\hat\psi_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle \\ = \big(\langle \Psi_{N;0}|\hat\psi^\dagger_\sigma(\boldsymbol{r})\tau(\boldsymbol{r})\hat\psi_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle\big)^*,\end{aligned} \tag{K2}$$

we deduce

$$\begin{aligned}\tau(\boldsymbol{r})n_\sigma(\boldsymbol{r}) &= 2\mathrm{Re}\big[\langle \Psi_{N;0}|\hat\psi^\dagger_\sigma(\boldsymbol{r})\tau(\boldsymbol{r})\hat\psi_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle\big] \\ &\quad -\frac{\hbar^2}{m_e}\langle \Psi_{N;0}|\big[\boldsymbol{\nabla}_{\boldsymbol{r}}\hat\psi^\dagger_\sigma(\boldsymbol{r})\big]\cdot\big[\boldsymbol{\nabla}_{\boldsymbol{r}}\hat\psi_\sigma(\boldsymbol{r})\big]|\Psi_{N;0}\rangle.\end{aligned} \tag{K3}$$

Making use of (see Eqs. (3) and (B16))

$$\langle \Psi_{N;0}|\hat\psi^\dagger_\sigma(\boldsymbol{r})\tau(\boldsymbol{r})\hat\psi_\sigma(\boldsymbol{r})|\Psi_{N;0}\rangle = \lim_{\boldsymbol{r}'\to\boldsymbol{r}} \tau(\boldsymbol{r})\,\varrho_\sigma(\boldsymbol{r}',\boldsymbol{r}) \tag{K4}$$

and Eq. (E13), from Eqs. (K3) and (43) we deduce [150] (below $\eta \downarrow 0$)

---

[146] We should emphasize that the singular nature of $\mathsf{n}_\sigma(k)$ at $k = k_{F;\sigma}$ necessitates (and this is signified by the principal-value nature of the integral on the RHS of Eq. (J6)) that integration by parts be carried out separately on the integrals over $[0, k_{F;\sigma} - 0^+]$ and $[k_{F;\sigma} + 0^+, \infty)$.

[147] The considerations by Farid (1999c) are specialized to uniform an isotropic systems of spin-less fermions or those in the paramagnetic state; however, the pertinent conclusions concerning $\mathsf{n}(k)$ arrived at by Farid (1999c) equally apply to $\mathsf{n}_\sigma(k)$.

[148] For *constant* number densities $\{n_\sigma\}$, $\widetilde{\mathsf{T}}^{\rm s}_{\sigma,\bar\sigma;\infty_2}(\boldsymbol{r}\|z)/z^2$ *identically* coincides with $\widetilde{\mathsf{T}}_{\sigma,\bar\sigma}(\boldsymbol{r};z)$ (see Eq. (G8)).

[149] By 'effective' we make provision for cases where Z_j may differ from the number of protons constituting the nucleus of the atom at $\boldsymbol{R}_j$ by the number of electrons that may have formed a tightly bound closed shell centred at $\boldsymbol{R}_j$ and as a result have not been taken account of in determining N in Eq. (20).

[150] We have $\Gamma^{(2)}(\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma') \equiv n_0^2\,\mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}'')$ (see Eq. (B21)). For the large-$\|\boldsymbol{r}-\boldsymbol{r}''\|$ asymptotic behaviour

$$
\begin{aligned}
\tau(\boldsymbol{r})\, n_\sigma(\boldsymbol{r}) &= -2u(\boldsymbol{r})\, n_\sigma(\boldsymbol{r}) - 2v_H(\boldsymbol{r};[n])\, n_\sigma(\boldsymbol{r}) \\
&-2\int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'') \sum_{\sigma'} \Big\{ \Gamma^{(2)}(\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma';\boldsymbol{r}\sigma,\boldsymbol{r}''\sigma') \\
&\qquad\qquad\qquad - n_{\sigma'}(\boldsymbol{r}'') n_\sigma(\boldsymbol{r}) \Big\} \\
&+\frac{2}{\hbar}\int_{-\infty}^{\infty} \frac{\mathrm{d}\varepsilon}{2\pi i}\, \mathrm{e}^{i\varepsilon\eta/\hbar}\, \varepsilon\, G_\sigma(\boldsymbol{r},\boldsymbol{r};\varepsilon) \\
&-\frac{\hbar^2}{m_e}\, \langle \Psi_{N;0} | \big[\boldsymbol{\nabla}_{\boldsymbol{r}} \hat{\psi}_\sigma^\dagger(\boldsymbol{r})\big] \cdot \big[\boldsymbol{\nabla}_{\boldsymbol{r}} \hat{\psi}_\sigma(\boldsymbol{r})\big] | \Psi_{N;0} \rangle. \qquad \text{(K5)}
\end{aligned}
$$

We have arranged the terms in this expression in such a way that it is also applicable to $d = 3$ and $v \equiv v_c$, where ϖ_κ as arising from $v_H(\boldsymbol{r};[n]) \equiv \varpi_\kappa + v_H(\boldsymbol{r};[n'])$ (see Eqs. (15) and (5)) exactly cancels that from $u(\boldsymbol{r})$ (see Eq. (11)). We therefore do *not* need to deal separately with the cases corresponding to $v \not\equiv v_c$ and $v \equiv v_c$ in $d = 3$. The appearance of $u(\boldsymbol{r})$ on the RHS of Eq. (K5) implies that $\tau(\boldsymbol{r}) n_\sigma(\boldsymbol{r})$ must be unbounded at $\boldsymbol{r} = \boldsymbol{r}_0$ if and only if $u(\boldsymbol{r})$ is so at $\boldsymbol{r} = \boldsymbol{r}_0$. The validity of this assertion relies on the consideration that *none* of the contributions on the RHS of Eq. (K5), except the first, can be unbounded.

Below we demonstrate the boundedness of all the contributions on the RHS of Eq. (K5) that follow the first term. For definiteness, we assume $d = 3$ and $v \equiv v_c$ and further that the electron-ion interaction is of the following form (for Z_j see above)

$$
u(\boldsymbol{r}) = \sum_j -Z_j\, v_c(\boldsymbol{r} - \boldsymbol{R}_j). \qquad \text{(K6)}
$$

We therefore view the $v_H(\boldsymbol{r};[n])$ on the RHS of Eq. (K5) as being replaced by $v_H(\boldsymbol{r};[n'])$ and $u(\boldsymbol{r})$ as not containing ϖ_κ (see above). One readily verifies that the second, third and fourth terms on the RHS of Eq. (K5) are bounded *everywhere*. For completeness, the abovementioned third and fourth terms are identical with $2\mathcal{B}''_\sigma(\boldsymbol{r},\boldsymbol{r})$ (see Eq. (F113)) and $2\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r})$ (see Eq. (E5)) respectively.

In order to investigate the behaviour of the last term on the RHS of Eq. (K5), we need to establish the behaviour of $\boldsymbol{\nabla}_{\boldsymbol{r}} \hat{\psi}_\sigma(\boldsymbol{r})$. To this end we point out that (as mentioned above, here we consider $d = 3$) with

$$
\mathsf{G}(\boldsymbol{r}-\boldsymbol{r}') \equiv \frac{-1}{4\pi\, \|\boldsymbol{r}-\boldsymbol{r}'\|}, \qquad \text{(K7)}
$$

$$
f(\boldsymbol{r}) = \int \mathrm{d}^3 r'\; \mathsf{G}(\boldsymbol{r}-\boldsymbol{r}')\, g(\boldsymbol{r}') \qquad \text{(K8)}
$$

is the solution of

$$
\nabla^2_{\boldsymbol{r}} f(\boldsymbol{r}) = g(\boldsymbol{r}). \qquad \text{(K9)}
$$

Making use of $\boldsymbol{\nabla}_{\boldsymbol{r}} \mathsf{G}(\boldsymbol{r}-\boldsymbol{r}') \equiv -\boldsymbol{\nabla}_{\boldsymbol{r}'} \mathsf{G}(\boldsymbol{r}-\boldsymbol{r}')$, on application of the divergence theorem from Eq. (K8) we obtain

$$
\boldsymbol{\nabla}_{\boldsymbol{r}} f(\boldsymbol{r}) = \int \mathrm{d}^3 r'\; \mathsf{G}(\boldsymbol{r}-\boldsymbol{r}')\, \boldsymbol{\nabla}_{\boldsymbol{r}'} g(\boldsymbol{r}'). \qquad \text{(K10)}
$$

From the Heisenberg equation of motion for the annihilation operator $\hat{\psi}_\sigma(\boldsymbol{r}t)$ (see Eq. (E6); see also footnote 44) we have

$$
\tau(\boldsymbol{r})\hat{\psi}_\sigma(\boldsymbol{r}) = i\hbar\, \frac{\mathrm{d}}{\mathrm{d}t} \hat{\psi}_\sigma(\boldsymbol{r}t)\Big|_{t=0} - u(\boldsymbol{r})\hat{\psi}_\sigma(\boldsymbol{r}) - \widehat{U}_\sigma(\boldsymbol{r}0), \qquad \text{(K11)}
$$

where

$$
\widehat{U}_\sigma(\boldsymbol{r}t) := \sum_{\sigma'} \int \mathrm{d}^d r''\; v(\boldsymbol{r}-\boldsymbol{r}'')\, \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}''t)\hat{\psi}_{\sigma'}(\boldsymbol{r}''t)\hat{\psi}_\sigma(\boldsymbol{r}t), \qquad \text{(K12)}
$$

which in the case of $d = 3$ and $v \equiv v_c$, is a bounded operator. With $\tau(\boldsymbol{r})$ as defined in Eq. (3), from Eq. (K11) in conjunction with Eq. (K10) we readily obtain

$$
\begin{aligned}
\boldsymbol{\nabla}_{\boldsymbol{r}} \hat{\psi}_\sigma(\boldsymbol{r}) = &\ \frac{2m_e}{i\hbar}\frac{\mathrm{d}}{\mathrm{d}t} \int \mathrm{d}^3 r'\; \mathsf{G}(\boldsymbol{r}-\boldsymbol{r}')\, \boldsymbol{\nabla}_{\boldsymbol{r}'} \hat{\psi}_\sigma(\boldsymbol{r}'t)\Big|_{t=0} \\
&+ \frac{2m_e}{\hbar^2} \int \mathrm{d}^3 r'\; \mathsf{G}(\boldsymbol{r}-\boldsymbol{r}') \boldsymbol{\nabla}_{\boldsymbol{r}'} \left[u(\boldsymbol{r}')\hat{\psi}_\sigma(\boldsymbol{r}')\right] \\
&+ \frac{2m_e}{\hbar^2} \int \mathrm{d}^3 r'\; \mathsf{G}(\boldsymbol{r}-\boldsymbol{r}') \boldsymbol{\nabla}_{\boldsymbol{r}'} \widehat{U}_\sigma(\boldsymbol{r}'0). \qquad \text{(K13)}
\end{aligned}
$$

With $u(\boldsymbol{r})$ as defined in Eq. (K6), from Eq. (K13) we observe that the most singular contribution to $\boldsymbol{\nabla}_{\boldsymbol{r}} \hat{\psi}_\sigma(\boldsymbol{r})$ is due to the following function which originates from the second term on the RHS of Eq. (K13); making use of Eqs. (K6) and (K7), for this contribution we have

$$
\begin{aligned}
\int \mathrm{d}^3 r'\; \mathsf{G}(\boldsymbol{r}-\boldsymbol{r}')[\boldsymbol{\nabla}_{\boldsymbol{r}'} u(\boldsymbol{r}')]\hat{\psi}_\sigma(\boldsymbol{r}') = \frac{-e^2}{(4\pi)^2\epsilon_0} \sum_j Z_j \\
\times \int \mathrm{d}^3 r'\; \frac{1}{\|\boldsymbol{r}-\boldsymbol{r}'-\boldsymbol{R}_j\|}\, \frac{\boldsymbol{r}'}{\|\boldsymbol{r}'\|^3}\, \hat{\psi}_\sigma(\boldsymbol{r}'+\boldsymbol{R}_j). \qquad \text{(K14)}
\end{aligned}
$$

The boundedness of this expression is established by demonstrating that for $\boldsymbol{r} \to \boldsymbol{R}_J$, for some J, the contribution of the most singular integral on the RHS of Eq. (K14), namely that corresponding to $j = J$, is bounded. This is achieved by equating $\boldsymbol{r}$ with $\boldsymbol{R}_J$ and considering a small spherical volume V_0 centred around the origin $\boldsymbol{r}' = \boldsymbol{0}$, for which holds:

$$
\begin{aligned}
\int_{V_0} \mathrm{d}^3 r'\; \frac{\boldsymbol{r}'}{\|\boldsymbol{r}'\|^4}\, \hat{\psi}_\sigma(\boldsymbol{r}'+\boldsymbol{R}_J) \approx \hat{\psi}_\sigma(\boldsymbol{R}_J) \\
\times \int_{V_0} \mathrm{d}^3 r'\; \frac{\boldsymbol{r}'}{\|\boldsymbol{r}'\|^4} \equiv \boldsymbol{0}. \qquad \text{(K15)}
\end{aligned}
$$

---

of $\mathsf{g}_{\sigma,\sigma'}(\boldsymbol{r},\boldsymbol{r}'')$ pertaining to uniform and isotropic systems see Appendix F, § F.1.d. We further note that the third term on the RHS of Eq. (K5) is identical with $2\mathcal{B}''_\sigma(\boldsymbol{r},\boldsymbol{r})$ (see Eqs. (F113) and (F112)) and the fourth term identical with $2\mathcal{D}_\sigma(\boldsymbol{r},\boldsymbol{r})$ (see Eq. (E13)).

Hereby we have demonstrated that the last term on the RHS of Eq. (K5) is bounded.

We have thus shown that $\tau(\boldsymbol{r})n_\sigma(\boldsymbol{r})$ is unbounded *only* there where $u(\boldsymbol{r})$ is unbounded, that is at the set of points $\{\boldsymbol{R}_j\}$. For $\boldsymbol{r}$ in the close vicinity of $\boldsymbol{R}_j$, from Eq. (K5) we therefore deduce the following asymptotic expressions:

$$\tau(\boldsymbol{r})n_\sigma(\boldsymbol{r}) \sim -2u(\boldsymbol{r})n_\sigma(\boldsymbol{r}) \sim -2u(\boldsymbol{r})n_\sigma(\boldsymbol{R}_j), \quad \text{when } \boldsymbol{r} \to \boldsymbol{R}_j. \tag{K16}$$

Expressing $\boldsymbol{r}$ in terms of its spherical polar coordinates (r, φ, θ), with the origin being centred at $\boldsymbol{r} = \boldsymbol{R}_j$, the asymptotic differential equation in Eq. (K16) implies that

$$\frac{\mathrm{d}}{\mathrm{d}r} n_\sigma(\boldsymbol{r})\Big|_{\boldsymbol{r}=\boldsymbol{R}_j} = -\frac{m_e e^2 Z_j}{2\pi\epsilon_0\hbar^2}\, n_\sigma(\boldsymbol{R}_j), \tag{K17}$$

from which we deduce that

$$n_\sigma(\boldsymbol{r}) \sim n_\sigma(\boldsymbol{R}_j) - \frac{m_e e^2 Z_j\, n_\sigma(\boldsymbol{R}_j)}{2\pi\epsilon_0\hbar^2}\, \|\boldsymbol{r} - \boldsymbol{R}_j\| \quad \text{when } \boldsymbol{r} \to \boldsymbol{R}_j. \tag{K18}$$

The results in Eqs. (K17) and (K18) coincide with those obtained earlier by other workers (Kato 1957, Bingel 1963, Steiner 1963, Pack and Brown 1966) and are referred to as the *cusp* conditions for $n_\sigma(\boldsymbol{r})$. Our approach in this Appendix is more transparent than those in the latter references. □

Some frequently-used notation

$\sim$	$f(x) \sim g(x)$ for $x \to x_0$ (say, $x_0 = \infty$) implies $f(x)/g(x) \to 1$ for $x \to x_0$
o	A Landau's symbol (E. G. H. Landau); $f(x) = o\big(g(x)\big)$ for $x \to x_0$ implies $f(x)/g(x) \to 0$ for $x \to x_0$
$\mathcal{O}$	A Landau's symbol (E. G. H. Landau); $f(x) = \mathcal{O}\big(g(x)\big)$, there exists a constant C such that $\vert f(x)\vert \le C\vert g(x)\vert$
$a \to b$	a approaches b
$a \rightharpoonup b$	b substitutes a
$a \rightleftharpoons b$	a and b are interchanged
$\Vert.\Vert$	Cartesian norm in d dimensions
s	Used as *subscript*, indicative of SSDA; e.g., $\varrho_{\mathrm{s};\sigma}$ denotes the SSDA of ϱ_σ
s	A compound index, characterizing the single-particle excitations of the *interacting* system; *cf.* $f_{s;\sigma}(\boldsymbol{r})$ (see Eq. (18))
ς	A compound index, in general characterizing the single-particle excitations of the *non*-interacting system; *cf.* $\varphi_{\varsigma;\sigma}(\boldsymbol{r})$ (see Eq. (56))
s	Spin of fermions, with multiplicity $2\mathsf{s}+1$
σ	A spin index (one out of $2\mathsf{s}+1$ indices)
$\bar{\sigma}$	The *set* of $2\mathsf{s}$ spin indices complimentary to σ; for $\mathsf{s} = \frac{1}{2}$, $\sigma =\uparrow$ implies $\bar{\sigma} =\downarrow$
N	$\sum_\sigma N_\sigma$, total number of fermions in the GS
N_σ	Number of fermions whose spin index is σ
$N_{\bar{\sigma}}$	$N_{\bar{\sigma}} = N - N_\sigma \equiv \sum_{\sigma' \ne \sigma} N_{\sigma'}$
d	The dimension of the spatial space
u	The local external potential
v	The two-body interaction potential
v_c	The two-body Coulomb potential in $d = 3$
ε	Real-valued energy parameter
z	Complex-valued energy parameter; unless otherwise stated, $\mathrm{Im}(z) \ne 0$
$\widetilde{f}(z)$	Analytic continuation of $f(\varepsilon)$ into the *physical* Riemann sheet; *cf.* $\Sigma_\sigma(\varepsilon)$ and $\widetilde{\Sigma}_\sigma(z)$
$\bar{\mathsf{f}}$	Fourier transform with respect to $\boldsymbol{r}$ of $\mathsf{f}(\boldsymbol{r})$
$\bar{\bar{\mathsf{f}}}$	Normalized $\bar{\mathsf{f}}$, according to $\bar{\bar{\mathsf{f}}}{:=}\bar{\mathsf{f}}/e_0$ where $e_0{:=}(2/r_s^2)$ Ry (see Eq. (103))
$\bar{\bar{\mathsf{g}}}$	Fourier transform with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$ of $\mathsf{g}(\boldsymbol{r}, \boldsymbol{r}')$
$\bar{\bar{\bar{\mathsf{g}}}}$	Normalized $\bar{\bar{\mathsf{g}}}$, according to $\bar{\bar{\bar{\mathsf{g}}}}{:=}\bar{\bar{\mathsf{g}}}/e_0$ where $e_0{:=}(2/r_s^2)$ Ry (see Eq. (103))
$\underline{\mathsf{h}}$	The 'Wigner transform' of $\mathsf{h}(\boldsymbol{r}, \boldsymbol{r}')$; $\underline{\mathsf{h}}(\boldsymbol{\rho}, \boldsymbol{\zeta}) \equiv \mathsf{h}(\boldsymbol{r}, \boldsymbol{r}')$, where $\boldsymbol{\rho} \equiv \boldsymbol{r} - \boldsymbol{r}'$, $\boldsymbol{\zeta} \equiv \frac{1}{2}(\boldsymbol{r} + \boldsymbol{r}')$
F^{h}	$F^{\mathrm{h}}(\Vert\boldsymbol{r} - \boldsymbol{r}'\Vert) \equiv F(\boldsymbol{r}, \boldsymbol{r}')$ corresponding to homogeneous *and* isotropic GSs; $F^{\mathrm{h}} \equiv F^{\mathrm{hi}}$
$F^{\mathrm{h}\neg\mathrm{i}}$	$F^{\mathrm{h}\neg\mathrm{i}}(\boldsymbol{r} - \boldsymbol{r}') \equiv F(\boldsymbol{r}, \boldsymbol{r}')$ corresponding to homogeneous but *not* isotropic states

LIST OF SOME ABBREVIATIONS

AS	Asymptotic series
GF	Green function; if not explicitly specified, the single-particle GF
GS	Ground state
LHS	Left-hand side
RHS	Right-hand side
RPA	Random-phase approximation
SE	Self-energy
SSD	Single-Slater-determinant
SSDA	Single-Slater-determinant approximation

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Errata concerning the published version of this work [*Phil. Mag.* B **82**, 1413-1610 (2002)]:

— On the third line of the paragraph on p. 1424, "(Anderson 1959, Gutzwiller 1963, Hubbard 1963, Ruijgrok 1962, Kanamori 1963)" should be "(Anderson 1959, Ruijgrok 1962, Gutzwiller 1963, Izuyama, *et al.* 1963, Hubbard 1963, Kanamori 1963)".

— In equation (106) on page 1456, "$\frac{\varepsilon_{\bar{k}}^{(0)}}{e_0}$" and "$\frac{1}{2}\bar{k}^2$" should be separated by "$\equiv$".

— On the LHS of equation (113) on page 1459, "$\hbar$" should be suppressed.

— On the 6th line of equation (199) on page 1483, "v^2" should be "$v(\boldsymbol{r}-\boldsymbol{r}'')$".

— On the 7th line of equation (199) on page 1483, "v^2" should be "$v^2(\boldsymbol{r}-\boldsymbol{r}'')$".

— In equation (223) on page 1494, "${}_2F_1(-\frac{1}{2}-m, 1; \frac{3}{2}-m; \frac{1}{\Delta^2\varepsilon^2})$" should be "${}_2F_1(\frac{1}{2}-m, 1; \frac{3}{2}-m; \frac{1}{\Delta^2\varepsilon^2})$".

— On the LHS of equation (227) on page 1495, "$(\varepsilon + i\eta)$" should be "$(\varepsilon \pm i\eta)$".

— On page 1495, 7th line below equation (227), "$(\varepsilon + i\eta)$" should be "$(\varepsilon \pm i\eta)$".

— On the LHS of equations (234a) and (234b) on page 1498, "$\overline{\Sigma}_\sigma$" should be "$\widetilde{\overline{\Sigma}}_\sigma$".

— On page 1523, "ϱ" on the RHS of the expression for Π_σ should be "$\wp$".

— On page 1533, last line of footnote 114, "$\varepsilon_{\bar{\boldsymbol{k}};\sigma}$" should be "$\varepsilon_{\boldsymbol{k};\sigma}$".

— On page 1547, on the 3rd line below equation (D10), "considering" should be "consider".

— On page 1572, on the 2nd line below equation (F97), "$\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'; \boldsymbol{r}_1''\sigma_2', \boldsymbol{r}_2''\sigma_2')$" should be "$\Gamma^{(2)}(\boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2'; \boldsymbol{r}_1''\sigma_1', \boldsymbol{r}_2''\sigma_2')$".

— On page 1587, on the 2nd line above equation (F161), "(F154)" should be "(F157)". □

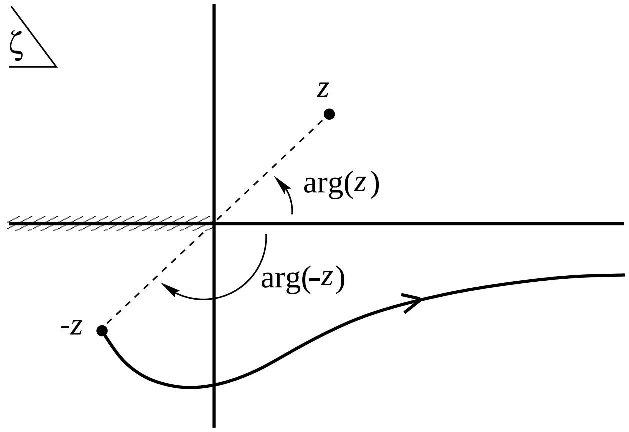

FIG. 1. The contour of integration in the complex ζ plane corresponding to the integral representation of the exponential-integral function $\mathrm{Ei}(z)$ as defined in Eq. (I3). The shaded part of the real axis indicates that the branch of the multi-valued function $\mathrm{Ei}(z)$ (viewed as a function of $-z$) relevant to our considerations, that is the 'principal' branch, is specified by the requirement $-\pi < \arg(-z) < \pi$. This aspect is directly associated with $\ln(-z)$ in Eq. (I4), with ln being the principle branch of the logarithm function.

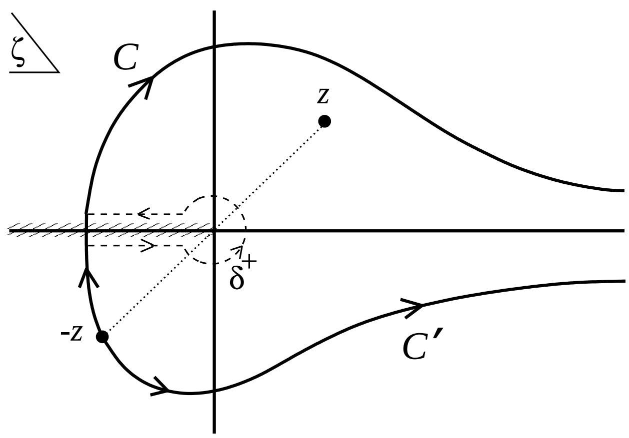

FIG. 2. The contours C and C' of integration in the complex ζ plane corresponding to $\mathcal{J}_C(z)$, as defined in Eq. (I5), and $\mathcal{J}_{C'}(z) \equiv \mathrm{Ei}(z)$, as introduced in Eq. (I3), respectively. The non-vanishing value of the integral of $\exp(-\zeta)/\zeta$ along contour δ^+, depicted by broken line, establishes that $\mathcal{J}_C(z)$ *cannot* be identified with $\mathrm{Ei}(z)$; see Eq. (I6).

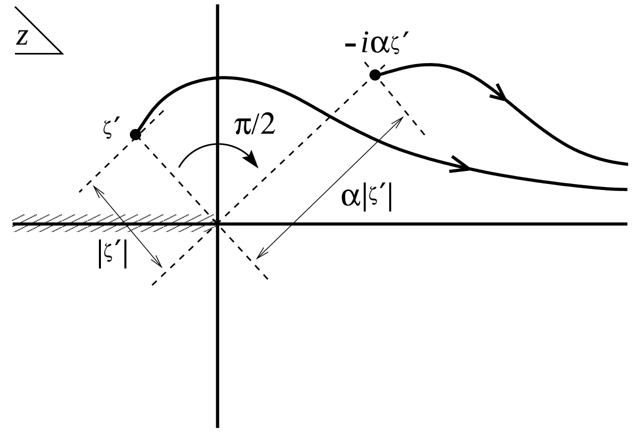

FIG. 3. In expressing $\mathcal{I}_1(\zeta';\alpha)$ as defined in Eq. (I1), through a process of transformation of the integration variable z, in terms of the exponential-integral function $\mathrm{Ei}(i\alpha\zeta')$, account has to be taken of the fact that this transformation can give rise to violation of the requirement $-\pi < \arg(-i\alpha\zeta') < \pi$ (see caption of Fig. 1). The transformation corresponding to an instance where ζ' is located in the second quadrant of the complex z plane and α is a positive constant is shown.

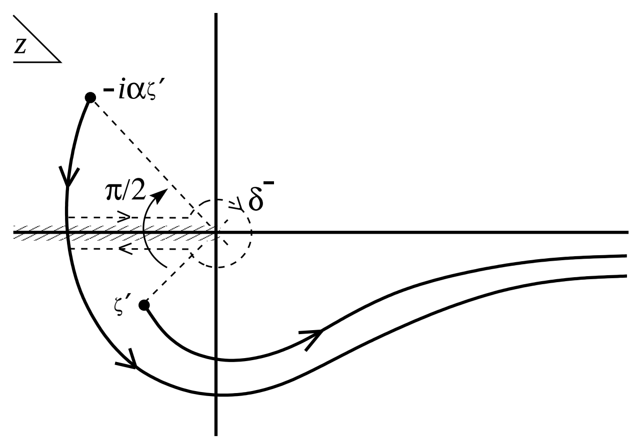

FIG. 4. Similar to Fig. 3, except that ζ' is located in the third quadrant of the complex z plane. With reference to the caption of Fig. 2, it is seen that, for $\alpha > 0$, transformation of the integration variable as described in the text does not allow direct identification of $\mathcal{I}_1(\zeta';\alpha)$ with $-\mathrm{Ei}(i\alpha\zeta')$; integration of $\exp(-z)/z$ along contour δ^-, depicted by means of the broken line, reveals the difference between the two functions (see Eq. (I7)).

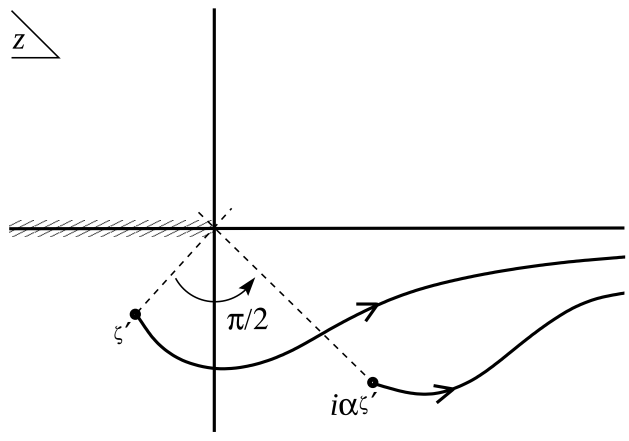

FIG. 5. Similar to Fig. 4, except that it concerns the transformation of the integration variable, that is z, in an attempt to express $\mathcal{I}_2(\zeta';\alpha)$, with $\alpha > 0$, in terms of $\mathrm{Ei}(-i\alpha\zeta')$ (see Eq. (I8)).

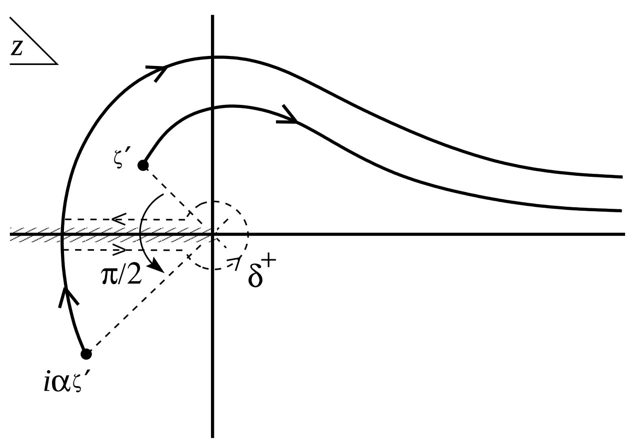

FIG. 6. Similar to Fig. 3, except that it concerns the transformation of the integration variable, that is z, in an attempt to express $\mathcal{I}_2(\zeta';\alpha)$, with $\alpha > 0$, in terms of the $\mathrm{Ei}(-i\alpha\zeta')$ (see Eq. (I8)).