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Chapter 3

Ground and Low-Lying Excited States of Interacting Electron Systems; A Survey and Some Critical Analyses*

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Abstract

In this contribution we deal with a number of theoretical aspects concerning physics of systems of interacting electrons. Our discussions, although amenable to appropriate generalisations, are subject to some limitations. To name, we deal with systems of spin-less fermions — or those of spin-*compensated* fermions with spin —, with nondegenerate ground states, and those in which relativistic effects are negligible; we disregard ionic motions and deal with "normal" (not superconducting, for instance) systems that are in addition free from randomly distributed impurities. We restrict our considerations to the absolute zero of temperature. The Green and response functions feature in our theoretical considerations. Here we give especial attention to the analytic properties of these functions for complex values of energy. We discuss how, both fundamentally and from the practical viewpoint, ground and low-lying excited-states properties can be obtained from these correlation functions. Characterising low-lying excited states by means of elementary excitations, we deal with both those that are particle-like (the Landau quasi-particles) and those that are

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*Dedicated to the memories of Dr Caroline P. Bammel, née Hammond, Fellow and Lecturer in Classics of Girton College and Reader in Early Church History of the University of Cambridge, United Kingdom, and Dr Dr Ernst Bammel, Reader Emeritus in Early Christian and Jewish Studies of the University of Cambridge and Professor of Theology of the University of Münster, Federal Republic of Germany.

collective (plasmons, excitation in the *total* distribution of electrons). We devote some space to discussions concerning the domain of validity and breakdown of the many-body perturbatiou theory, specifically that for the single-particle Green function and the self-energy operator. Extensive analysis of the asymptotic behaviour of *dynamic* correlation functions in the limits of small and large energies reveal the significance of the Kohn-Sham-like Hamiltonians within the context of the many-body perturbation theory. In view of this, at places we pay especial attention to a number of the existing density-functional theories (including the ones for the single-particle reduced density matrix and time-dependent external potentials). We discuss in some detail a number of issues that are specific to the (phenomenological) Landau Fermi-liquid theory and their justification within the framework of the many-body perturbation theory. In doing so we touch upon a number of characteristic features specific to Fermi-liquid (as oppsed to marginal Fermi- and Luttinger-liquid) systems. Finally, we put one particular approximation scheme for the self-energy operator, known as the the GW scheme, under magnifying glass and observe it in many of its facets.

1. Introduction

The two-body Coulomb interaction amongst electrons can never justifiably be neglected in any theoretical consideration. It can however happen that its main effects may be subsumed in some one-body effective potential. Whether such effective theories can be constructed, and if so, how the residual interaction can be accounted for, are questions that are addressed within the framework of the many-body theory.

The need for an effective description of interacting systems arises for two reasons, of which one is perceptual and the other practical. The former is related to the way in which we are able to conceive of things.[1] Perceptually, one may be able to conceive of the correlated state of a two-particle system, however beyond this one does not seem to have the ability to forming concrete ideas concerning the state and of what it possibly can represent. On the practical side, the larger the number of the particles, the greater the effort that has to be spent in order to calculate a correlated state and extract from

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[1] "Thinking in terms of one / Is easily done — / One room, one bed, one chair, / One person there, / Makes perfect sense; one set / Of wishes can be met, / One coffin filled. // But counting up to two / Is harder to do; / For one must be denied / Before it's tried." [Philip Larkin, *Counting*, September? 1955]

it information concerning properties of the system. Whence the popularity of such effective one-body theories as the Hartree and Hartree–Fock and a wealth of other alternative methods. But from where do these methods derive their formal justification? We shall, amongst other things, address this question in the present work.

Before entering into details, we should clarify what we exactly mean by "properties" of a system. A "property" can be the expectation value of a certain operator with respect to some eigenstate of the Hamiltonian of the system under consideration, or it can be an average of such expectation values over some ensemble of eigenstates of the mentioned Hamiltonian, such as a thermal ensemble. For keeping our discussions transparent, in this work we shall be dealing with non-degenerate ground states (GSs) and properties corresponding to these (there are many realistic many-electron systems that possess such GSs). It turns out that knowledge concerning GSs of such systems is sufficient for deducing not only the GS properties, but also those of the excited states. Our knowledge concerning the excited states will not be complete, however: we will not be able in principle to relate a calculated excited-state property to any definite excited eigenstate.

Green functions (GFs) are mathematical constructs that formally come close to meet both of the demands indicated above. An n-particle GF (think of $n \simeq 1$) pertaining to an N-particle system (possibly $N \simeq 10^{24}$) may be considered as an effective wave function of this system in that as far as certain properties of the system are concerned, it yields exactly the same results as the exact wave function, however contrary to the wave function it cannot directly inform us about certain other properties. This is often an advantage, for from the experimental point of view there are always a very limited number of properties that are *or* can be probed and all the additional information about the system may at all not be conductive to a better understanding of the processes underlying the observed phenomena. In the present work we will mainly be interested in the single-particle Green function G (Sec. 4) as well as some reduced forms of the two-particle GF, such as the density-density correlation function χ and the polarisation function P (Sec. 8).

Consider the single-particle GF which is the expectation value of a time-ordered product of two field operators with respect to the N-electron *ground state* of the system (Sec. 4). It is well-known that poles[2] of this function along

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[2] Until we have specified different types of singularities in Sec. 2.1, we shall follow the common practice and for all types of singularities employ the designation "pole".

the energy axis coincide with the energies of the $(N \pm 1)$-electron states of the system as measured from the energy of the N-electron GS, i.e., the one-particle excitation energies. In general, for extended systems comprised of large numbers of electrons, excited states are highly (nearly) degenerate: from simple dimensional considerations it follows that for a system of linear dimension L, the separations between the energy levels scale like L^{-2} (Landau and Lifshitz 1980a, p. 14). As a consequence of this massive exact or almost exact degeneracy of the excited states of the many-electron systems, it follows that for systems in the thermodynamic limit the description of the excitation spectra, such as the one contained in the spectral function corresponding to the single-particle GF (Subsecs. 4.4 and 6.1), in terms of isolated *exact* excitations is no longer meaningful, for the reason that individual excitation energies cannot be experimentally resolved. In fact from the mathematical point of view, the procedure of taking the thermodynamic limit leads to the "smearing" of poles into branch cuts (see Sec. 2). In practice, in particular in interpreting experimental observations, it is common to identify the sharp and prominent features in the spectra with excitation energies of new types of particles, quasi particles (QPs), such as (Abrikosov, Gorkov and Dzyaloshinski 1963, Pines and Nozières 1966, Ashcroft and Mermin 1981, Landau and Lifshitz 1980b, Kittel 1986): "excitons", "magnons", "plasmons", "polarons", "polaritons", "quasi electrons", "quasi holes", "rotons", etc. (see Secs. 6.1, 6.3 and 8.7). The width of one such sharp peak in a spectrum will then be associated with the degree of de-coherence, or lifetime, of the corresponding excitation. The broadness of a peak can be accounted for by assigning an imaginary part to the corresponding excitation energy.

The *complex* "poles" of correlation functions (see Secs. 2, 6 and 8) that are associated with the excitation energies of a system in the thermodynamic limit, are *not* necessarily approximate devices introduced for the sake of convenience in reproducing the broad spectra. This is clarified by the following observation: In taking the thermodynamic limit, correlation functions become in general ill defined *if* the external energy parameter ε in the respective expressions is kept to be real-valued. On the other hand, no problem can arise when the thermodynamic limit is taken while the energy parameter is made into a complex variable, z (Subsec. 2.2). This process is not reversible in that upon approaching the real energy axis from the complex plane, subsequent to having taken the thermodynamic limit, correlation functions are seen *not* to have maintained their poles of the pre-thermodynamic-limit stage. Rather, these poles are turned into branch cuts or branch points (Sec. 2). Analytic continuation through these cuts reveals that the experimentally observed peaks correspond to poles of the pertinent analytically-continued functions (Subsec. 6.1); it is then said that these complex poles are located on a *non-physical* Riemann sheet (RS), (Subsec. 2.2). These poles, with non-vanishing imaginary parts, *cannot* lie on the physical RS (Subsec. 2.2): owing to a reflection property with respect to the real energy axis, occurrence of poles on the physical RS (excluding hereby the real energy axis itself) implies violation of the principle of causality.

For low excitation energies, and in particular for systems that are classified as Fermi-liquid[3] systems (Sec 6.3), Landau QPs (Landau 1957a — see: Abrikosov and Khalatnikov 1959, Abrikosov, Gorkov, and Dzyaloshinski 1963, Nozières 1964, Pines and Nozières 1966, Platzman and Wolff 1973, Baym and Pethick 1978, Landau and Lifshitz 1980b, Rickayzen 1980, Negele and Orland 1988, Fulde 1995) turn out to be well defined: for a homogeneous degenerate Fermi liquid and small external energies ε — as measured with respect to the Fermi energy ε_F —, the imaginary part of the self-energy (SE) operator $\Sigma(\varepsilon)$ behaves like $\sim' (\varepsilon-\varepsilon_F)^2$, implying that for sufficiently small $|\varepsilon-\varepsilon_F|$, Landau QPs are fairly long-lived excitations. Such property gives rise to some universal behaviour in the thermodynamic properties of the corresponding systems at low temperatures (Luttinger 1960). For instance the behaviour $\gamma T+\delta T^3\ln(T)$, with γ and δ constants, is particular to the specific heat at low temperatures (T) of Fermi liquids (Amit, Kane and Wagner 1967, 1968). The low-energy behaviours of SEs of systems classified as *marginal* Fermi liquids (Varma, Littlewood, Schmitt-Rink, Abrahams and Ruckenstein 1989), or *Luttinger* liquids (Footnote 5 in Luttinger 1961, Luttinger 1963, Mattis and Lieb 1965, Haldane 1981; see Voit (1994)) differ from that just presented.[4]

Our above description of Fermi-liquid systems suggests that these must have gap-less excitations. In this sense semiconductors and insulators cannot be classified as Fermi-liquid systems (see however further on). Examples of *normal* Fermi liquids are (Pines and Nozières 1966): ^3He above 4 mK,

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[3] Here "liquid" is the short for "quantum liquid", to be distinguished from a "classical liquid". The distinction between the two stems from the fact that in quantum liquids the *degeneracy* of the constituent particles (that, in the present case, their equilibrium distribution is a Fermi-Dirac distribution) plays a significant role. For both types of liquids, however, the interparticle interaction is of crucial import (and in this "liquids" are distinct from "gases").

[4] From the present point of view, even $\mathrm{Im}\Sigma(\varepsilon\to\varepsilon_F)\sim'(\varepsilon-\varepsilon_F)^\sigma$, $\sigma>1$, or $\sim'(\varepsilon-\varepsilon_F)^\sigma\ln|\varepsilon-\varepsilon_F|$, $\sigma>1$, signify Fermi liquids (Farid 1999a).

conduction electrons in metals, semi-metals and heavily-doped semiconductors (Ashcroft and Mermin 1981, Kittel 1986). The Fermi-liquid theory in its original form (Landau 1957a, 1957b, 1959) had concerned homogeneous systems, however its underlying concepts admit generalisation to inhomogeneous systems (Luttinger 1960). Thus the routinely-calculated electronic band-structures in solids are nothing but energies that in some approximate framework are associated with the QP energies. The one-particle-like equations employed in these calculations are *often*[5] simplified forms of a Schrödinger-type equation for QPs (Sec. 6). The simplifications amount to replacing the energy-dependent non-Hermitian SE operator by a static Hermitian operator that in an effective way is supposed to take account of the interaction effects. In such *static* effective theories, QPs behave like non-interacting electrons (e.g., they have infinite lifetimes) with renormalised or effective parameters (such as an effective mass). Thus systems of particles of effective theories (such as the Hartree and Hartree–Fock theories — in general, "mean-field" theories) are by construction Fermi liquids (excluding anomalies), provided of course that they possess a Fermi surface which may be possibly multi-sheeted (Sec. 6). Hence systems that are known to have non-Fermi-liquid-like behaviour are beyond the reach of *static* effective theories (or, "band theories").

In this work we present a self-contained framework within which the single-particle Green function G of an interacting system can be determined (see Sec. 4). This function can be used to calculate a non-negligible number of properties corresponding to the GS of this system; these include all properties whose corresponding operators involve one-body terms, which may be *local* or *non-local* (Fetter and Walecka 1971, pp. 66 and 67). The expression for the GS total energy due to Galitskii and Migdal (1958) shows that even this quantity, which involves the *two-body* electron-electron interaction, can be fully expressed in terms of the single-particle GF (Subsec. 9.7). To calculate G it is necessary that we deal with a number of other correlation functions which, due to their physical significance, have been given specific names. These include the density-density correlation function χ, the polarisation function P, the dielectric function ϵ, the pair-correlation function g, the SE operator Σ and the vertex function Γ. In this work in addition to G we consider χ, P, g and Σ in some detail.

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[5] For very fundamental reasons, the one-particle Kohn-Sham (1965) (KS) equation does *not* belong to the category of approximate QP equations.

From a formal spectral representation for $G(\varepsilon)$, where ε denotes the external energy parameter which through the Fourier transform is reciprocal to the time parameter t, known as the Lehmann (1954) representation (Fetter and Walecka 1971), it becomes evident that the information concerning the one-particle excitation spectrum[6] of the interacting system is contained in $G(\varepsilon)$. However, for systems in the thermodynamic limit — which are systems of our main interest in the present work —, determination of $G(\varepsilon)$ must of necessity (see above) be based on that of $\widetilde{G}(z)$, with z a complex-valued energy variable, from which $G(\varepsilon)$ is obtained according to $G(\varepsilon) = \lim_{\eta\downarrow 0} \widetilde{G}(\varepsilon \pm i\eta)$, for $\varepsilon > \mu$ and $\varepsilon < \mu$; here μ stands for the "chemical potential" (see Subsec. 4.2). We refer to $\widetilde{G}(z)$ as the analytic continuation of $G(\varepsilon)$ into the physical RS of the complex z-plane (Subsec. 2.2). The many-valuedness of $\widetilde{G}(z)$ implies that there are other branches corresponding to $G(\varepsilon)$ which through analytic continuation of $G(\varepsilon)$ or $\widetilde{G}(z)$ across the branch cuts (Sec. 2) can be constructed; we denote all these other functions collectively by $\widetilde{\widetilde{G}}(z)$ and refer to them as analytic continuations of $G(\varepsilon)$ or $\widetilde{G}(z)$ into *non-physical* RSs. We consider the analytic properties of $\widetilde{G}(z)$ in the complex z-plane and present a so-called *bi-orthonormal* representation (Morse and Feshbach 1953, pp. 883–886, Layzer 1963) for it which is in terms of the left and right eigenvectors of a non-Hermitian operator $\widetilde{\mathcal{H}}_{qp}(z)$. We demonstrate this to be the "Hamiltonian" for the "Landau quasi-particles" (a "one-body" picture!). This "Hamiltonian" is general and its meaningfulness is independent of whether the system to which it corresponds is a Landau Fermi liquid or not.

The energy-dependent non-Hermitian term in $\widetilde{\mathcal{H}}_{qp}(z)$ is the SE operator $\widetilde{\Sigma}(z)$ which is the analytic continuation into the physical RS of the physical SE operator $\Sigma(\varepsilon)$; the correspondence between $\widetilde{\Sigma}(z)$ and $\Sigma(\varepsilon)$ is exactly the same as that between $\widetilde{G}(z)$ and $G(\varepsilon)$ presented above. In Sec. 5 we give a detailed discussion of the analytic properties of $\widetilde{\Sigma}(z)$.

In Sec. 6 we consider solutions of the one-particle Schrödinger-like equation corresponding to the above-mentioned QP "Hamiltonian" $\widetilde{\mathcal{H}}_{qp}(z)$. On the basis of some analytic property of $\widetilde{\Sigma}(z)$, we arrive at the conclusion that this Schrödinger-like equation either has solutions corresponding to QPs with real-valued energies or it has *no* solution. For obtaining solutions corresponding to QPs with complex-valued energies, the SE operator in the Schrödinger-like equation has to be replaced by an analytic continuation of $\Sigma(\varepsilon)$ into a

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[6] For the precise definition see Subsec. 4.1.

non-physical RS. This has significance for determining the complex-valued QP energies and their spectral "weights", which are in consequence also complex-valued. We discuss these issues in Sec. 6.1 under the heading "the quasi-particle approximation." To make contact with physics of real materials, we apply the results thus-far obtained to a system about which a great deal is known, namely the uniform-electron system. Thus we revisit some well-known theorems due to Migdal (1957) (Luttinger 1960) and Luttinger (1961) (Luttinger and Ward 1960), making appropriate distinction between the different branches of the functions that we encounter in the course of our analyses. Here we critically analyse a theorem due to Luttinger (1961) which has played an important role in characterising Fermi-liquid systems. We show that due to in particular one tacit assumption by Luttinger (1961), it is *not* necessary that non-Fermi-liquid behaviour in the low-temperature properties of a system should signal breakdown of the many-body perturbation theory (PT) for this system.

In Sec. 7 we briefly deal with various methods of determination of G and Σ. We give especial attention to the many-body PT. We present various ways in which a many-body perturbation expansion for G can break down (Subsecs. 7.4 and 7.4.1) and present a sufficient condition for the validity of the zero-temperature many-body PT. It turns out that provided the GS electronic density of the interacting system under consideration be pure-state non-interacting v-representable,[7] the zero-temperature many-body perturbation expansion in terms of the pertinent Kohn-Sham (1965) (KS) Hamiltonian does *not* break down (Farid 1997a, 1999b).[8]

In Subsec. 7.4.2 we present an argument, first advanced by Dyson (1952), which has shed much unfavourable light on the PT ever since its publication. In Subsec. 7.4.3, making use of some arguments and examples put forward by Simon (1970), we attempt to remove some of the misconceptions with regard to the domain of applicability of the many-body PT.

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[7] Briefly, non-interacting v-representability of the GS charge density n signifies that it can be reproduced as the GS charge density of a "non-interacting" Hamiltonian, the Kohn-Sham (1965) (KS) Hamiltonian; "pure-state" refers to the requirement that the GS of the KS Hamiltonian in question be a *single* Slater determinant. *All* physical densities are so-called ensemble v-representable. For a comprehensive review see (Dreizler and Gross 1990).

[8] We have to emphasise that by this we do *not* mean that a finite-order perturbation expansion in terms of the pertinent KS Hamiltonian should be sufficient for all purposes. "Breakdown" here refers to the condition in which predictions of the theory are not in accord with the actual facts *after summation over all the terms in the perturbation series*. In this light, a PT that predicts an actually insulating state to be metallic, has been subject to a breakdown.

In view of the importance of the dynamic screening effects in interacting systems, and in view of the important role that these play in the determination of G and Σ, in Sec. 8 we present the pertinent response functions, such as χ and P. Here we present a bi-orthonormal representation for $\widetilde{\chi}(z)$ in terms of the left and right eigenfunctions of a non-Hermitian operator. Our treatment here runs parallel to that for $\widetilde{G}(z)$ in Sec. 4. Here we derive an equation which is reminiscent of the QP equation in Sec. 6, whose solutions we show to be associated with the plasmon excitations in interacting systems. Again it turns out that this equation can only yield real-valued plasmon energies (which *may not* exist) and that for obtaining complex-valued plasmon energies it is required that $\chi(\varepsilon)$ be analytically continued into a non-physical RS. In this Section, through analysing the behaviour of $\chi(\varepsilon)$ and the related functions (such as $P(\varepsilon)$) at small and large values of $|\varepsilon|$, we expose the crucial role that the *ground-state* charge density plays in determining *dynamic* screening properties of interacting systems. This indirectly shows the merits of the KS Hamiltonian in applications of the many-body PT (see above and Sec. 7): It turns out that at the zeroth order of the PT, the response functions in the limit of large $|\varepsilon|$, yield the same results as is expected from the exact response functions. We further emphasise the close relationships between the ε-moments integrals of the branch-cut discontinuity (the "imaginary part") of the exact $\chi(\varepsilon)$ and such properties as the GS charge density and the electronic pair-correlation function. Here we consider the density-functional theory (DFT) for GSs (Hohenberg and Kohn 1964) and that for time-dependent external potentials (Runge and Gross 1984). We draw attention to the fact that within these frameworks the effect of the electron-electron interaction can rigorously be taken into account in describing such correlation functions as $\chi(\varepsilon = 0)$ and $\chi(\varepsilon \neq 0)$. We indicate some fundamental restriction within the framework of the time-dependent DFT that stands in the way of incorporating interaction effects in $\chi(\varepsilon)$ for *arbitrary* ε. Further, we expose the links between the moments expansion of $\chi(\varepsilon)$ (as a typical example from a large class of correlation functions) and the continued-fraction expansion of the branch-cut discontinuity of $\widetilde{\chi}(z)$. Truncated continued-fraction expansions have an interesting property in view of their association with the method of Gaussian quadrature for integration (Stoer aud Bulirsch 1980, pp. 142–151). This association is of utmost importance in connection with the ε-integrations that occur in the expressions that lead to correlation functions. We also present a plasmon-pole model for $\widetilde{\chi}(z)$. This model (Engel and Farid 1993) serves to illustrate a variety of concepts that we have encountered in the earlier Sections.

In recent years an approximation for the SE operator, referred to as the GW approximation (Hedin 1965), has attracted considerable amount of interest. In Sec. 9 we deal with this approximation. The *general* aspects concerning the exact SE operator, discussed in earlier Sections (Secs. 5, 7), are made explicit in Sec. 9. An aspect which we have *not* considered *in full detail* in Secs. 5, 7 (due to technical complications), concerns the large-$|\varepsilon|$ behaviour of $\Sigma(\varepsilon)$. In Sec. 9 we take up the task of explicitly calculating the first three terms in the asymptotic expansion of $\Sigma^{GW}(\varepsilon)$ for large $|\varepsilon|$. Both these and the first two energy moments of $\Sigma^{GW\prime\prime}(\varepsilon)$ — the branch-cut discontinuity of $\widetilde{\Sigma}^{GW}(z)$ — make explicit, for yet another time, how prominent the role played by the GS electron density $n(\mathbf{r})$ and the GS single-particle reduced density matrix $\rho(\mathbf{r},\mathbf{r}')$ is in the many-body theory. It turns out that as far as the mentioned terms in the asymptotic expansion of $\Sigma^{GW}(\varepsilon)$ and the energy moments of $\Sigma^{GW\prime\prime}(\varepsilon)$ are concerned, $\Sigma^{GW}(\varepsilon)$ is *almost* identical to $\Sigma^{G_0W_0}$ evaluated in terms of the G_0 and W_0 pertaining to a non-interacting Hamiltonian $\widehat{H}_0$ whose corresponding $n_0(\mathbf{r})$ and $\rho_0(\mathbf{r},\mathbf{r}')$ [the Dirac-Fock reduced density matrix] are identical to $n(\mathbf{r})$ and $\rho(\mathbf{r},\mathbf{r}')$, the latter pair pertaining to the fully interacting system. This makes us to turn our attention again to the DFT. It is seen that such a "non-interacting" Hamiltonian is an integral part of a DFT first considered by Gilbert (1975). Further, we present a list of references that covers research activities involving Σ^{GW} over a relatively long period of time — regrettably, due to limitation of space we restrict ourselves to works that in the main concern three-dimensional solids. Finally, given the fact that Σ^{GW} is merely an approximation to Σ, we briefly consider the question as to the extent to which Σ^{GW} can account for the electron-electron interaction effects. We are of the opinion that the overwhelming success of the GW approximation (GWA) in yielding accurate results for the low-lying single-particle *excitation energies* of semiconductors and insulators may be for a non-negligible part due to a cancellation of errors: that the inaccuracies due to G_0 and W_0 (almost invariably corresponding to the KS Hamiltonian in terms of the local-density approximation (LDA) for the exchange-correlation potential [Kohn and Sham 1965]) and those due to the GWA itself, largely cancel (Farid 1997a). We indicate the desirability of future detailed and systematic studies on the subject.

In Sec. 10 we summarise our work and present some conclusions. Of the two Appendices that follow Sec. 10, Appendix A concerns the (notational) conventions with regard to the representations that we employ in the present work, while Appendix B serves to emphasise the relationship between the asymptotic behaviour of a function of ε at large $|\varepsilon|$ on the one hand, and the behaviour of the inverse-Fourier transform of this function in the limit of small $|t|$ (t denotes the time) on the other. Following the Appendices, we have included two lists, one of mathematical symbols and the other of abbreviations and acronyms of the frequently-used words in the present work.

As is evident from this introduction, in our work we rely quite substantially on a variety of mathematical concepts. To make our text self-contained, we devote Sec. 2 to a brief exposition of these (Farid 1999a). In choosing the illustrative examples in this Section, we have endeavoured that these involve such elements as those which we encounter in the subsequent Sections of the present work. In Subsec. 2.4 we present the physical motivation for the concepts that we introduce in Subsecs. 2.1, 2.2 and 2.3.

2. Mathematical Preliminaries

In this work we frequently encounter a number of mathematical notions. This Section serves to make our text self-contained.

2.1. *Types of singularity*

A point at which a function of complex variable z, say $g(z)$, is not *analytic* (*analytic*, *regular* and *holomorphic* are interchangeable) is called a *singular* point of $g(z)$. Such singular point, say z_0, can be (Whittaker and Watson 1927, pp. 102 and 104; Titchmarsh 1939, pp. 89–95; Knopp 1945, pp. 117–139; Spiegel 1974, pp. 67, 68, 144 and 145) either *isolated* or *non-isolated*; z_0 is isolated if there exits a $\delta > 0$ such that within the circle $|z - z_0| = \delta$, z_0 is the only singular point of $g(z)$. Otherwise z_0 is *non-isolated*.

Singularity of $g(z)$ at *the point of infinity* corresponds to that of $g(1/\zeta)$ at $\zeta = 0$. A function which is analytic everywhere with the exception of the point of infinity, is referred to as *entire* or *integral* (thus $\exp(z)$ is entire).

A singularity can be *removable*; such singularity corresponds to a point z_0 at which $g(z)$ is *not* defined, but $\lim_{z\to z_0} g(z)$ exists. Thus $z = 0$ is a removable singularity of $g(z) := \sin(z)/z$.

Non-isolated singularities, such as *limiting* or *accumulation* points of a sequence of poles, are *not* classified as poles and thus are considered as *essential* singularities. For instance the sequence of poles of $g(z) := \sum_{n=0}^{\infty} 1/(n!\,[1 + a^{2n} z^2])$, with $a > 1$, have $z = 0$ as their limiting point: $z = 0$ is a non-isolated, and thus an essential, singularity of $g(z)$; this function has no Laurent (or Taylor) series expansion through any region which has $z = 0$ as its *interior*.

Let $g(z)$ be single-valued throughout a region D which contains the point z_0 at which $g(z)$ is singular. Suppose the *principal part* of the Laurent expansion of $g(z)$ around $z = z_0$ terminates with the term $a_{-n}/(z - z_0)^n$. In such case, z_0 is called a *pole* of order n of $g(z)$. Poles are thus by definition *isolated* singularities. Functions whose singular points consist in a *finite* set of poles are called *meromorphic*.

If the principal part of the Laurent expansion of $g(z)$ around $z = z_0$ does not terminate (i.e., if n in $a_{-n}/(z - z_0)^n$ goes to infinity), z_0 is an *isolated essential singularity* of $g(z)$. A theorem due to Casorati, Weierstrass and Picard (Knopp 1945, p. 128) establishes that for any two positive numbers δ_1 and δ_2, and any complex number C, there exists a z inside the circle $|z - z_0| = \delta_1$, with z_0 an isolated essential singularity of $g(z)$, for which holds $|g(z) - C| < \delta_2$. That is, by approaching z_0 in different ways, $g(z)$ can take on any arbitrary value. As an example, consider $g(z) := \exp(z)$ which has an isolated essential singularity at the point of infinity. One can easily verify that by an appropriate choice for r and θ in $r\exp(i\theta) =: \zeta$, $g(1/\zeta)$ indeed attains any arbitrary value as $r \to 0$.

According to a theorem due to Cauchy, but commonly referred to as the Liouville theorem (Whittaker and Watson, 1927, p. 105), a function that is analytic everywhere, *including* the point of infinity, must be a constant; when one allows unbounded functions in the class of analytic functions, a generalised version of the "Liouville theorem" establishes that *only* finite-order polynomials can be analytic everywhere. Thus all *entire* functions, with the exception of finite-order polynomials, have essential singularities at the point of infinity.

Branch points belong to the class of singular points and concern multi-valued functions. Suppose $g(z)$ is one such function. By traversing a closed contour which circumscribes only one branch point of $g(z)$, one obtains a value different from the initial value upon arriving at the starting point, indicating that the initial branch of $g(z)$ is interchanged by a different branch; for a branch point z_0 of order p, the original branch is recovered after completion of p full rotations along the mentioned contour. Thus $(z - z_0)^{1/3}$ has a third-order branch point at $z = z_0$. Functions can possess branch points of infinite order; for $\ln(z)$, $z = 0$ is one such point.

2.2. *Many-valued functions: Physical and non-physical Riemann sheets*

An n-valued function of complex variable z (Whittaker and Watson 1927, pp. 96–98; Titchmarsh 1939, pp. 138–164, Knopp 1947, pp. 93–118) over domain D may be thought of as consisting of n branches of single-valued functions $\tilde{f}_i(z)$, $i = 1, 2, \ldots, n$, over D. Alternatively, this n-valued function can be considered as a single-valued function over the extended domain consisting of a union of n replicas of D; since these domains signify the same region on the complex plane, they are distinguished as being on different sheets, *Riemann sheets* (RS), of the complex plane. We denote by $\mathcal{F}(z)$ the union of all $\tilde{f}_i(z)$'s over the larger domain of n RSs. Riemann sheets corresponding to $\mathcal{F}(z)$ are connected together along the branch cuts of $\mathcal{F}(z)$. We denote that branch of $\mathcal{F}(z)$ which has direct physical significance (see further on) by $\tilde{f}(z)$. Consequently, we refer to $\tilde{f}(z)$ as "$\mathcal{F}(z)$ on the physical RS", and to other branches as "$\mathcal{F}(z)$ on the non-physical RSs". In the text of the present work we denote *all* the latter branches by $\tilde{\tilde{f}}(z)$.

Let ε be real-valued. Let there be the function $f(\varepsilon)$ defined over $\Delta := (\varepsilon_1, \varepsilon_2)$ such that

$$\tilde{f}(z) \rightarrow f(\varepsilon) \quad \text{as} \quad z \rightarrow \varepsilon \,. \tag{1}$$

Suppose that $\tilde{f}(z)$ approaches $f(\varepsilon)$ *uniformly*[9] when $z \rightarrow \varepsilon$, i.e. that for a given $\delta_1 > 0$ there exists a $\delta_2 > 0$, *independent* of ε inside Δ, such that for $|y| < \delta_2$ (with y real-valued), $|\tilde{f}(\varepsilon + iy)) - f(\varepsilon)| < \delta_1$. In such an event $\tilde{f}(z)$ is called *the* analytic continuation of $f(\varepsilon)$ into the complex z-plane; a function like $f(\varepsilon)$ to which an analytic function $\tilde{f}(z)$ in the above sense corresponds, is referred to as being "analytically continuable" into the complex z-plane.[10] It is important that in the case the interval Δ is part of a branch cut of $\tilde{f}(z)$, the process of analytic continuation of $\tilde{f}(z)$ from, say, the upper half-plane can be extended, through the real interval Δ, into the lower half-plane. The thus-obtained function coincides with a branch of $\mathcal{F}(z)$ which is different from $\tilde{f}(z)$. Thus if $\tilde{f}(z)$ were the *physical* branch, the new branch would be a non-physical branch. One could equivalently state tbat in moving z from the upper half-plane through the branch cut into the lower half-plane, we have moved from the physical RS into a non-physical one. See Fig. 1.

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[9] The condition of *uniformity* can be shown, *a posteriori*, to be redundant: the existence of the limit in Eq. (1), with $f(\varepsilon)$ *continuous* over Δ, implies uniformity of the limit (see: Streater and Wightman 1964, p. 75).

[10] Some analytic functions, referred to as *lacunary* functions, *cannot* be analytically continued from inside to outside of their domain of definition (Whittaker and Watson 1927, p. 98).

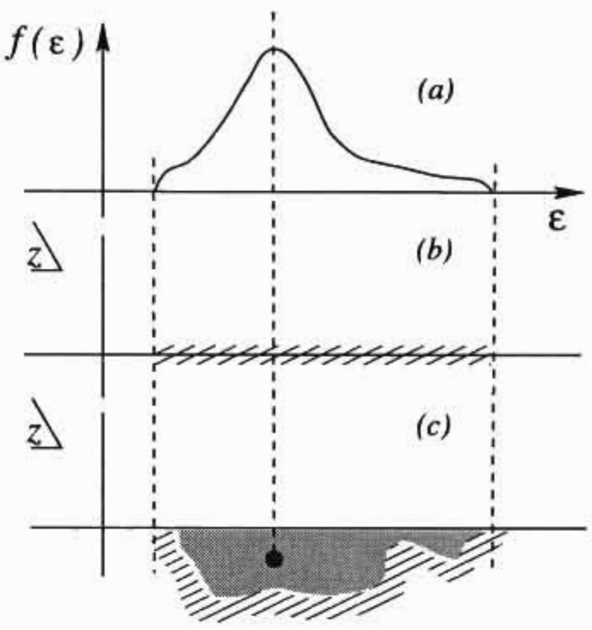

Fig. 1. The peak of function $f(\varepsilon)$ along the *real* energy axis (a) may be thought of as corresponding to a *complex* pole of the analytic continuation of $f(\varepsilon)$ into the ***physical*** Riemann sheet (RS) of the complex z-plane, $\widetilde{f}(z)$. On the physical RS of the z-plane (b) there is no pole to be found, only a branch cut (the shaded section of the ε-axis). In (c), part of the physical RS is "removed" (indicated by the grey area which is part of the ***non-physical*** RS which is *directly* accessible from the upper-half of the physical RS). The peak of $f(\varepsilon)$ is seen to correspond to a pole of $\mathcal{F}(z)$ (indicated by the bold dot) on the non-physical RS. For the mathematical details see Subsec. 2.2.

An example should clarify the above notions. Consider $f(\varepsilon) := \ln(\varepsilon)$, with $\varepsilon > 0$. It can be shown that $\ln(z) =: \widetilde{f}(z)$ is the analytic continuation of $f(\varepsilon)$ from the positive real axis ($\equiv \Delta$) into the z-plane.[11] Now if $f(\varepsilon)$ denoted some physical quantity (say, the frequency-dependent optical conductivity as measured experimentally), $\widetilde{f}(z)$, defined above, would coincide with the physical branch of $\mathcal{F}(z)$, i.e. it were $\mathcal{F}(z)$ on the physical RS. Let $\mathrm{Ln}_n(z) := \ln|z| + i\{\arg(z) + 2\pi n\}$ with $-\pi \le \arg(z) < \pi$. The function $\mathcal{F}(z)$ in the present case coincides with the union of $\mathrm{Ln}_n(z)$ for *all* n (i.e., n negative, zero and positive), and $\widetilde{f}(z) \equiv \mathrm{Ln}_{n=0}(z)$. If we were given $\mathcal{F}(z)$ and asked to find the physical branch, i.e. $\widetilde{f}(z)$, we needed to find that $\mathrm{Ln}_n(z)$ which yielded $f(\varepsilon)$ when $z \to \varepsilon > 0$ (see Eq. (1) above). This procedure of selecting the physical branch out of many (possibly, infinitely many) branches of a many-valued function is *not* subject to arbitrariness. This is owing to a uniqueness theorem

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[11] It is somewhat unfortunate that customarily all *standard* functions, such as ln, sin, cos, etc., whether their arguments be real or complex, are denoted by the same symbol.

(Titchmarsh 1939, p. 139): two analytic functions that are defined on the same region of the complex plane (in the present case, the entire complex plane, with the exception of the origin), and are equal on a line (here, the positive real axis), or over a set of points that has a point of accumulation, are *identical.* In the present case, for instance, this theorem implies that there exists *only* one n (which we know to be $n = 0$) for which $\lim_{z\to\varepsilon>0} \mathrm{Ln}_n(z) = f(\varepsilon)$ can hold.

If we choose z in the argument of $\widetilde{f}(z)$ to satisfy $\mathrm{Re}(z) < 0$, while let $\mathrm{Im}(z)$ change from some positive (negative) value to some negative (positive) value, we will achieve that $\widetilde{f}(z)$ is analytically continued into $\mathrm{Ln}_{n=1}(z)$ ($\mathrm{Ln}_{n=-1}(z)$). For $\mathrm{Im}(z) \downarrow 0$ we have $\lim_{z\to\varepsilon}\{\widetilde{f}(z)-\widetilde{f}(z^*)\}/(2i) = 0, \pi$, depending on whether $\mathrm{Re}(z) > 0$ or $\mathrm{Re}(z) < 0$. The non-vanishing value for the case $\mathrm{Re}(z) < 0$ is the consequence of the branch cut of $\widetilde{f}(z)$ along the negative real axis; this branch cut connects the two branch points of $\ln(z)$, one at $z = 0$ and the other at $1/z = 0$.

2.3. *Series and asymptotic series*

If $g(z)$ is analytic at $z = z_0$, then, owing to the fact that notion of analyticity is defined by means of a pair of *differential equations* (Riemann-Cauchy's), there is an *open* region D which has z_0 as its interior and in which $f(z)$ is analytic. Within a circle centred around z_0 and embedded inside D, $g(z)$ can be represented in terms of a Taylor series (Whittaker and Watson 1927, pp. 93 and 94, Titchmarsh 1939, pp. 83 and 84): $g(z) = \sum_{n=0}^{\infty} a_n(z - z_0)^n$, with $a_n := (1/n!)d^n g(z)/dz^n|_{z=z_0}$. The coefficients a_n are unique. We have explicitly presented this series for bringing out the fact that for $g(z)$, and thus *all* functions that like $g(z)$ are analytic at $z = z_0$, there exists a finite region around z_0 where $\{(z - z_0)^n \mid n = 0, 1, \ldots\}$ forms a *complete* set of basis functions. For functions that possess an *isolated* singularity at $z = z_0$, this set is *not* complete, but can be made into one by allowing n to take on negative, in addition to zero and positive, integer values. The series in terms of this extended set of basis functions is the well-known Laurent series (Whittaker and Watson 1927, p. 100, Titchmarsh 1939, pp. 89–91); the series involving the negative values of n is referred to as the *principal part* of the Laurent expansion.

For $g(z)$ which has a non-isolated singularity at $z = z_0$, *no* Laurent expansion can be constructed centred around $z = z_0$ for a region that contains z_0 as interior. However, by excluding the circular region around z_0 that contains all singularities of $g(z)$ of which z_0 is the limiting point, it is possible to construct a Laurent expansion around z_0 which is valid for some non-vanishing region. As an example consider $g(z) := \sum_{n=0}^{\infty} 1/(n![1+a^{2n}z^2])$, with $a > 1$. In Subsec. 2.1 we have mentioned that $z = 0$ is a non-isolated singularity of $g(z)$. For $|z| > 1$, $g(z)$ has the following Laurent series expansion (Whittaker and Watson, 1927, p. 105): $g(z) = \sum_{n=1}^{\infty}(-1)^{n+1}\exp(1/a^{2n})/z^{2n}$.

A specific feature of Taylor and Laurent expansions is their *uniformity*: once their validity has been established for $z = r\exp(i\theta)$, corresponding to a *fixed* value of θ, it follows that they are valid for *all* $\theta \in [0, 2\pi)$.

Branch points belong to the set of possible singular points of $g(z)$. However, with z_0 a branch point of $g(z)$, $g(z)$ does *not* allow for a *uniform* representation, such as a Laurent expansion, in a neighbourhood of z_0. To use our above terminology, the set $\{(z-z_0)^n \mid \ldots, -2, -1, 0, 1, 2, \ldots\}$ does *not* form a complete basis for representing functions, in a neighbourhood of z_0, that possess a branch point at z_0. Nonetheless, this set has a significance in the context of *asymptotic* expansion of $g(z)$ for $z \rightarrow z_0$. We note that if two branch points of $g(z)$ that are connected by a branch cut can be circumscribed by a circle of finite radius, then $g(z)$ can be represented by a Laurent series valid for some region exterior to this circle. If, on the other hand, one of these branch points is the point of infinity, it is no longer possible to construct a uniform series expansion around any point on the branch cut. Thus, for instance, it is not possible to obtain for $\ln(z)$ a uniform series expansion around $z = 0$, or some point along the negative real axis.

Asymptotic expansions (Whittaker and Watson 1927, Ch. VIII, Copson 1965, Lauwerier 1977, Dingle 1973) are with respect to some so-called *asymptotic sequencc.* An asymptotic sequence, e.g. $\{\phi_n(z)|n = 0, 1, \ldots\}$, has the property that in the asymptotic region, specified through $z \rightarrow z_0$, has the property that $\phi_{n+1}(z)/\phi_n(z) \rightarrow 0$; this is denoted by $\phi_{n+1}(z) = o(\phi_n(z))$. Thus $\{(z-z_0)^n \, |n = 0, 1, \ldots\}$ represents an asymptotic sequence for $z \rightarrow z_0$. A theorem from the theory of asymptotic analysis states that (Copson 1965, pp. 5 and 6, Lauwerier 1977, p. 13) if a given function, say $g(z)$, has an asymptotic expansion [in Poincaré's sense — the sense according to which *all* our asymptotic expansions in subsequent sections are carried out] of order M with respect to some given asymptotic sequence, say $\{\phi_n(z)\}$, meaning that $g(z) = \sum_{n=0}^{M} a_n\phi_n(z) + o(\phi_M(z))$, then the coefficients $\{a_n|n = 0, 1, \ldots, M\}$ of the asymptotic expansion are *unique*. For $M = \infty$ this series does *not* need to be convergent (even for $z \rightarrow z_0$), however; in fact in some texts (e.g., Whittaker and Watson 1927) the designation "asymptotic series" is reserved for those series which are both asymptotic (in the sense of being in terms of an asymptotic sequence) *and* divergent. Nor is it necessary that a function has a *uniform* asymptotic series. Functions with *non-uniform* asymptotic series for $z \to z_0$, are those which possess different asymptotic series for different sectors of the z-plane around z_0. Consider, for instance, $g(z) := \exp(z) + \exp(-z)\tanh(1/z)$ which has the following asymptotic series for $z \to 0$: $g(z) \sim 2\cosh(z) \sim 2 + z^2 + \cdots$, for $\mathrm{Re}(z) > 0$, and $g(z) \sim 2\sinh(z)$ $\sim 2z + z^3/3 + \ldots$, for $\mathrm{Re}(z) < 0$ (Lauwerier 1977, p. 11). This, that in different sectors around a point in the complex plane a function can have different asymptotic expansions with respect to the same asymptotic sequence, is referred to as the *Stokes phenomenon* (Watson 1952, Berry 1966, 1989, 1990, 1991a,b, Dingle 1973, Boyd 1990, McLeod 1992).

The Taylor series of analytic functions based on point z_0 are *convergent* asymptotic expansions for $z \to z_0$. It can be shown that even to divergent asymptotic series corresponding to the asymptotic sequence $\{(z - z_0)^n | n = 0, 1, \ldots\}$ an analytic function can be associated of which the given (divergent) series is the asymptotic expansion (Lauwerier 1977, pp. 12–14). Thus, for instance, after Borel (or Euler) transformation (Whittaker and Watson 1927, pp. 154 and 155, Lauwerier 1977, pp. 45–50, Negele and Orland 1988, pp. 373–376, Dingle 1973, pp. 405–408) of the divergent series $f(z) := \sum_{n=0}^{\infty}(-1)^n n! z^n$, one obtains the $f_B(z) := \sum_{n=0}^{\infty}(-1)^n z^n = (1 + z)^{-1}$. Through the Borel back transformation (Lauwerier 1977, p. 49, Negele and Orland 1988, p. 374) of $f_B(z)$, $\overline{f}_B(z) := \int_0^{\infty} dx\ \exp(-x) f_B(xz)$, one obtains a function, i.e. $\overline{f}_B(z)$, which is analytic in the sector $-\pi < \arg(z) < \pi$ of the z-plane; it can be shown that $\overline{f}_B(z) \equiv z^{-1}\exp(1/z)\Gamma(0, 1/z)$ where $\Gamma(a, z)$ denotes the incomplete Gamma function (see Davis, P.J., in Abramowitz and Stegun 1972, p. 260). Through replacing $f_B(xz)$ by its formal geometric series expansion $1 - xz + (xz)^2 - \cdots$ and evaluating the above integral term-by-term, the original divergent series is recovered. We observe that the divergence of the original asymptotic series is closely associated with the restricted sector of the z-plane around $z = 0$ for which $\overline{f}_B(z)$ is analytic. We point out that divergent asymptotic series can be useful, as they yield very accurate results when they are truncated at some optimal order (see Copson 1965, Dingle 1973).

In our considerations concerning analytic properties of $\widetilde{\Sigma}(k_F; z)$ (see Subsecs. 2.4 and 6.3), we will establish that this function has a branch point at $z = \varepsilon_F$. This indicates that not only there can be no Taylor expansion for

$\widetilde{\Sigma}(k_F; z)$ around $z = \varepsilon_F$, the asymptotic expansion of this function with respect to the asymptotic sequence $\{(z-\varepsilon_F)^n \,|\, n = 0, 1, \ldots\}$ will be divergent when expansion is continued to infinite order (see above); the possibility of convergence of this series would contradict non-analyticity of $\widetilde{\Sigma}(k_F; z)$ at $z = \varepsilon_F$.

2.4. *Physical motivation*

Below by means of a simple example we motivate our above detailed considerations. This example embodies many of the aspects that are shared by the correlation functions pertaining to many-particle systems, several of which we shall encounter in the subsequent Sections of the present work.

Consider $f(\varepsilon; N, \Omega) := \Omega^{-1} \sum_{s=1}^{\mathcal{N}} \{\theta(\varepsilon_s - e_0) - \theta(\varepsilon_s - e_1)\}/(\varepsilon_s - \varepsilon)$, $\varepsilon_{s+1} > \varepsilon_s$, whose form in essential ways is similar to that in, e.g., Eqs. (11) and (100). Here e_0 and e_1 are finite constants for which we assume $e_0 < \varepsilon_s < e_1$ for some values of s; N, Ω indicate that f is a function of the number N of the particles as well as the volume Ω of the system. In the "thermodynamic limit" (corresponding to $N \to \infty$, $\Omega \to \infty$ and a finite concentration $\mathsf{C} := N/\Omega$), f is a function of C, and thus we denote it by $f(\varepsilon; \mathsf{C})$. For finite N and Ω, it is seen that $f(\varepsilon; N, \Omega)$ has poles at all ε_s in the interval $[e_0, e_1]$.

If $f(\varepsilon; N, \Omega)$ described some property of a physical system, the quantities ε_s could be viewed as energies of the natural modes of that system. Since these modes are infinite in number, $\mathcal{N}$ is infinitely large.[12] Moreover, if this system were in free space (i.e., not placed inside an impenetrable box), the spectrum would be partly continuous, and thus s would be in part a continuous variable. To avoid unnecessary complications, we restrict our present considerations to confined systems. Since, however, $\mathcal{N}$ is infinitely large, the "spectrum" of such a confined system *must* at least have one *accumulation* point; this follows from the Bolzano-Weierstrass theorem (Whittacker and Watson 1927, pp. 12 and 13). Thus some singular points ε_s of $f(\varepsilon; N, \Omega)$, $\varepsilon_s \in [e_0, e_1]$, may not be *isolated* but *non-isolated* (see Subsec. 2.1). As an example, consider the energies of the *bound states* of the Hydrogen atom. Since these converge towards zero as the principal quantum number n approaches infinity, *zero* is an accumulation point in the spectrum of the bound states of Hydrogen.

We now take the "thermodynamic limit". Since upon doing so, in general (i.e. disregarding some possible "gaps" in the spectrum), $|\varepsilon_{s+M} - \varepsilon_s| \downarrow 0$ for any *finite* M, the function $f(\varepsilon; N, \Omega)$ will be ill-defined for real values

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[12] This necessarily follows from the *completeness* of the eigenstates of such systems — described by self-adjoint energy operators.

of ε inside $[e_0, e_1]$ — as ε may be "pinched" by two adjacent poles. This necessitates that the "thermodynamic limit" be taken not of $f(\varepsilon; N, \Omega)$ but of $\widetilde{f}(z; N, \Omega) \equiv f(z; N, \Omega)$ with $\mathrm{Im}(z) \neq 0$, unless $\mathrm{Re}(z)$ happens to be inside some gap. We observe that, in general (i.e., excluding the cases where ε is inside some possible gap or $\varepsilon \notin [e_0, e_1]$), evaluation of the thermodynamic limit can give rise to a meaningful $f(\varepsilon; \mathrm{C})$ provided this be defined as the limit of $\widetilde{f}(z; \mathrm{C})$ with $|\mathrm{Im}(z)| \to 0$. For $\widetilde{f}(z; \mathrm{C})$ to qualify as the *physical* branch — as $\widetilde{f}(z; \mathrm{C})$ is only one branch out of possibly infinite number of branches of a many-valued function —, it is required that in regions where $f(\varepsilon; \mathrm{C})$ is well-defined (for instance inside the gaps, or, in the present case, in the regions $\varepsilon < e_0$ and $\varepsilon > e_1$), the two functions $\widetilde{f}(\varepsilon; \mathrm{C})$ and $f(\varepsilon; \mathrm{C})$ coincide (see Subsec. 2.2 where we considered $f(\varepsilon) := \ln(\varepsilon)$, $\varepsilon > 0$).

Suppose now that poles of $\widetilde{f}(z; N, \Omega)$ are uniformly distributed and that this property persists into the "thermodynamic limit", with the density of poles per unit energy approaching the constant value $A\Omega$. Suppose further that e_0 and e_1 remain finite in the "thermodynamic limit". Under these conditions, the sum in the definition of $\widetilde{f}(z; N, \Omega)$ transforms into an integral, which in the present case can be evaluated analytically. We have: $\widetilde{f}(z; N, \Omega) \cong A \int_{e_0}^{e_1} d\varepsilon'/(\varepsilon' - z)$ $= A\{\ln(z - e_1) - \ln(z - e_0)\} =: \widetilde{f}(z; \mathrm{C})$. In Fig. 2 we depict the analytic structure of this function. We point out that here $\ln(z)$ stands for the *principal* branch of the logarithm function. That this choice indeed renders $\widetilde{f}(z; \mathrm{C})$ the *physical* branch is seen as follows:

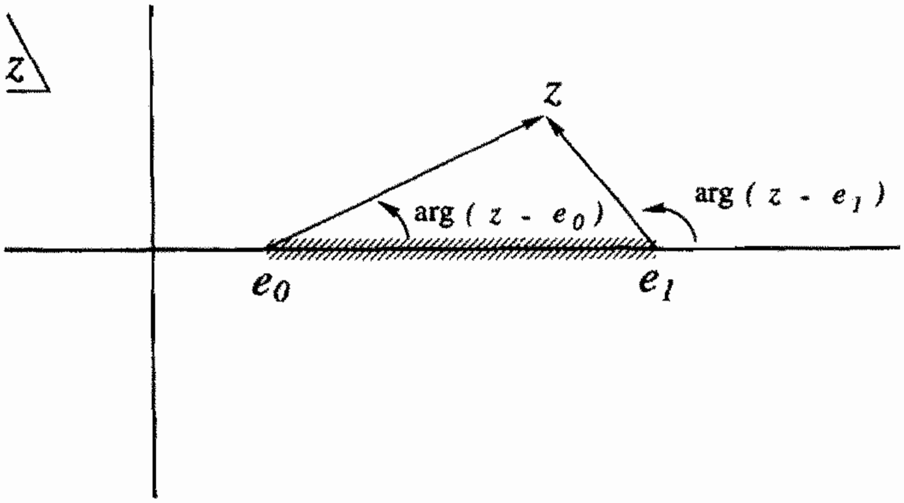

Fig. 2. The complex z-plane and the analytic structure of $\widetilde{f}(z; \mathrm{C}) := A\{\ln(z - e_1) - \ln(z - e_0)\}$. The shaded part of the real axis indicates the branch cut of $\widetilde{f}(z; \mathrm{C})$ which joins the branch points e_0 and e_1.

Consider $\widetilde{f}(\varepsilon \pm i\eta; \mathsf{C}) \equiv A \int_{e_0}^{e_1} d\varepsilon'/(\varepsilon' - \varepsilon \mp i\eta)$, with $\eta \downarrow 0$. Making use of the Cauchy theorem, or what *here* is the same, $1/(\varepsilon' - \varepsilon \mp i\eta) = \mathcal{P}\{1/(\varepsilon' - \varepsilon)\} \pm i\pi\delta(\varepsilon' - \varepsilon)$, with $\mathcal{P}$ the Cauchy principal value, one readily obtains $\widetilde{f}(\varepsilon \pm i\eta; \mathsf{C}) = A\{\ln|e_1 - \varepsilon| - \ln|e_0 - \varepsilon|\} \pm i\pi A\theta(\varepsilon - e_0)\theta(e_1 - \varepsilon)$. Hence for $\varepsilon < e_0$ and $\varepsilon > e_1$, the "physical" $\widetilde{f}(\varepsilon \pm i\eta; [\mathsf{C}])$, $\eta \downarrow 0$, must be real valued, while for $e_0 < \varepsilon < e_1$, $\widetilde{f}(\varepsilon + i\eta; \mathsf{C}) - \widetilde{f}(\varepsilon - i\eta; \mathsf{C}) = 2\pi i A$; the interval $[e_0, e_1]$ is the branch cut of $\widetilde{f}(z; \mathsf{C})$. These conditions can be verified to be fulfilled, provided the above logarithm functions with *complex* argument are the principal branch of the logarithm function.

Let us now for the sake of better understanding the details, determine some analytic continuations of the above $\widetilde{f}(z; \mathsf{C})$ into non-physical RSs. In accordance with our convention, we denote these "non-physical" extensions collectively by $\widetilde{\widetilde{f}}(z; \mathsf{C})$. Let $\widetilde{g}(z) := A\{\mathrm{Ln}_1(z - e_1) - \ln(z - e_0)\}$. It is easily verified that for $e_0 < \varepsilon < e_1$, $\lim_{\eta\downarrow 0}\{\widetilde{f}(\varepsilon + i\eta; \mathsf{C}) - \widetilde{g}(\varepsilon - i\eta)\} = 0$, which implies that $\widetilde{g}(z)$ is the analytic continuation of $\widetilde{f}(z; \mathsf{C})$ from the upper-half plane through the branch cut $[e_0, e_1]$ into the lower-half plane of a non-physical RS (it is helpful to use Fig. 2 as a visual aid). Thus $\widetilde{g}(z)$ qualifies to be denoted by $\widetilde{\widetilde{f}}(z; \mathsf{C})$ — see Subsec. 2.2. Similarly, it can be shown that as long as $\varepsilon \in (e_0, e_1)$, for $\widetilde{h}(z) := A\{\mathrm{Ln}_{-1}(z - e_1) - \ln(z - e_0)\}$ holds $\lim_{\eta\downarrow 0}\{\widetilde{f}(\varepsilon - i\eta; \mathsf{C}) - \widetilde{h}(\varepsilon + i\eta)\} = 0$, i.e. $\widetilde{h}(z)$ is the analytic continuation of $\widetilde{f}(z; \mathsf{C})$ from the lower-half plane through the branch cut $[e_0, e_1]$ into the upper-half plane of another non-physical RS (thus also $\widetilde{h}(z)$ qualifies to be denoted by $\widetilde{\widetilde{f}}(z; \mathsf{C})$). Since $\widetilde{g}(z) \not\equiv \widetilde{h}(z)$, the two corresponding RSs are different, which is another way of stating that $\widetilde{g}(z)$ and $\widetilde{h}(z)$ are two different branches of $\mathcal{F}(z; \mathsf{C})$.

Although the transition to the "thermodynamic limit" leads to condensation of poles into branch cuts, in some cases and in certain representations, the singularities of correlation functions of systems in the thermodynamic limit can show up as *poles*. The conservation laws corresponding to the symmetries of the problem are responsible for this, namely owing to the existence of conserved quantities, one has the possibility to decompose the physical processes in the interacting system (i.e. the virtual transition events) into disjoint classes, each class corresponding to a specific (set of) allowed value (values) for the conserved quantity (quantities);[13] this can be achieved through using the bases corresponding to the irreducible representations of the

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[13] The possibility of fixing more than one conserved quantity depends on whether the associated symmetry groups commute.

underlying symmetry group(s). For instance, in a uniform system — with continuous translation symmetry —, the linear momentum in each virtual scattering event is conserved. For such a system, therefore, scattering events can be classified in terms of the wave-vector **k** transferred. Specialising our above example to a uniform system, the sum over s can be replaced by one over **k** (see Appendix A); clearly, for a given **k** (which, because of being a conserved quantity, is physically well-defined) and $e_0 < \varepsilon_{\mathbf{k}} < e_1$, we have to do with a simple pole at $z = \varepsilon_{\mathbf{k}}$. If the underlying symmetry of the system is a discrete translation symmetry (such as is the case in infinite crystals), wavevector is conserved only up to a reciprocal-lattice vector (RLV). Nevertheless, since in this case $\sum_s(\ldots)$ can be replaced by $\sum_{\mathbf{k}\in 1\mathrm{BZ}} \sum_{\mathbf{G}}(\ldots)$ and the inner summation is over the *discrete* set of RLVs, for a given reduced wavevector **k** inside the first Brillouin zone (1BZ) we have to do with poles; in the thermodynamic limit $\sum_{\mathbf{k}\in 1\mathrm{BZ}}$ transforms into an integral, giving rise to "smearing" of these poles into branch cuts. We should emphasise that not always use of an appropriate representation will help exposing the singularities of a correlation function as poles. This happens when, in interacting systems, the functions under consideration describe higher than the first-order interaction processes. For instance, when second-order processes are taken into account, we encounter expressions that involve *two* nested summations: $\sum_s \sum_{s'}(\ldots)$. It follows that even if we represent this as $\sum_{\mathbf{k}} \sum_{\mathbf{G}}\{\sum_{\mathbf{k}'} \sum_{\mathbf{G}'}(\ldots)\}$, the inner $\mathbf{k}'$-sum, which in the thermodynamic limit transforms into an integral, changes the possible poles due to the summand of the $\mathbf{G}'$-sum into branch cut(s) so that singling out processes corresponding to the reduced wavevector **k** is of no avail. This simple consideration suggests that finite lifetimes of quasi-particles (in uniform and periodic systems) should originate from the second- and higher-order interaction processes (see Subsec. 6.4).

Before closing this section, we present an example which brings out the relevance of the above considerations to our subsequent discussions in the present work (see in particular Sec. 6). In Subsec. 6.3 we shall see that for a uniform-electron system, solution $z = z_s \equiv \varepsilon_k$ of $\widetilde{E}_k(z) = z$, with $\widetilde{E}_k(z) := \varepsilon_k^0 + \hbar\widetilde{\Sigma}(k; z)$, corresponds to the energy of a QP. Here $\varepsilon_k^0 := \hbar^2 k^2/(2m_e)$ and $\widetilde{\Sigma}(k; z)$ denotes the SE operator in the wave-vector representation (see Appendix A). Suppose for the QP energy ε_k holds $\mathrm{Im}\widetilde{\Sigma}(k; \varepsilon_k) \neq 0$. Then from the requirement $\widetilde{E}_k(z = \varepsilon_k) = \varepsilon_k$ it follows that ε_k *cannot* be real-valued. It can be shown that $\widetilde{E}_k(z^*) = \widetilde{E}_k^*(z)$ — reflection symmetry with respect to the real energy axis, Eq. (62) —, so that the existence of a QP with *complex-valued* "energy" ε_k

implies existence of a QP with "energy" ε_k^*. This is in violation of the principle of causality. This contradiction would be resolved if $\mathrm{Im}\widetilde{\Sigma}(k;\varepsilon_k) = 0$, in which case ε_k would correspond to an excitation with infinite lifetime, which contradicts our original assumption. Hence the only *complex* QP energies can lie on the non-physical RSs. For obtaining these energies, one has to solve $\widetilde{\widetilde{E}}_k(z) = z$.

3. Generalities

In this Section we introduce the Hamiltonian of the interacting system which we shall be considering throughout this work.

Consider the many-body Hamiltonian $\widehat{H}$ for spin-less electrons in the second-quantisation representation,

$$\widehat{H} := \widehat{T} + \widehat{U} + \widehat{V}\,, \tag{2}$$

where

$$\widehat{T} := \int d^3r\, \widehat{\psi}^\dagger(\mathbf{r}) \left[\frac{-\hbar^2}{2m_e}\nabla^2\right] \widehat{\psi}(\mathbf{r})\,, \tag{3}$$

$$\widehat{U} := \int d^3r d^3r'\, \widehat{\psi}^\dagger(\mathbf{r}) u(\mathbf{r},\mathbf{r}')\widehat{\psi}(\mathbf{r}')\,, \tag{4}$$

$$\widehat{V} := \frac{1}{2}\int d^3r d^3r'\, \widehat{\psi}^\dagger(\mathbf{r})\widehat{\psi}^\dagger(\mathbf{r}') v_c(\mathbf{r}-\mathbf{r}')\widehat{\psi}(\mathbf{r}')\widehat{\psi}(\mathbf{r}) \tag{5}$$

stand for the kinetic energy, the energy due to the external potential and the electron-electron interaction energy, respectively. In Eq. (5), $v_c(\mathbf{r}-\mathbf{r}') := e^2/(4\pi\epsilon_0\|\mathbf{r}-\mathbf{r}'\|)$ stands for the Coulomb potential[14] with e^2 the electron charge $-e$ (< 0) squared and ϵ_0 the vacuum permittivity. The operators $\widehat{\psi}^\dagger$, $\widehat{\psi}$ are, respectively, creation and annihilation field operators in the Schrödinger representation and satisfy the well-known fermion *anti-commutation* relations (Fetter and Walecka 1971, p. 19). The real symmetric function $u(\mathbf{r},\mathbf{r}')$ stands for the *external* potential which for the sake of generality we consider to consist of a *local* and a strictly *non-local* contribution, i.e.

$$u(\mathbf{r},\mathbf{r}') := v(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}') + w(\mathbf{r},\mathbf{r}')\,. \tag{6}$$

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[14] In principle one may choose some other appropriate two-body potential. Further, it should be realised that the *instantaneous* nature of $v_c(\mathbf{r}-\mathbf{r}')$ in Eq. (5) signifies the fact that $\widehat{H}$ has been written in the Coulomb gauge (Mahan 1981, pp. 60 and 66).

In the calculations concerning solids, where often ionic potentials are replaced by ***pseudo-potentials***, v and w correspond to respectively the local and non-local parts of the ionic pseudo-potentials (Hamann, Schlüter and Chiang 1979, Kerker 1980, Bachelet, Hamann and Schlüter 1982). We explicitly assume that $v(\mathbf{r})$ and the real symmetric $w(\mathbf{r}, \mathbf{r}')$ do not involve any differential operators acting on the functions of $\mathbf{r}$, and $\mathbf{r}'$, to their right sides. For later use we introduce

$$\begin{aligned} \widehat{U}_v &:= \int d^3r\, \widehat{\psi}^\dagger(\mathbf{r}) v(\mathbf{r}) \widehat{\psi}(\mathbf{r}) , \\ \widehat{U}_w &:= \int d^3r d^3r'\, \widehat{\psi}^\dagger(\mathbf{r}) w(\mathbf{r}, \mathbf{r}') \widehat{\psi}(\mathbf{r}') . \end{aligned} \tag{7}$$

4. The Single-Particle Green Function

In this Section we deal in some detail with the single-particle Green function G corresponding to the interacting system described by $\widehat{H}$ in Eq. (2). We give especial attention to the analytic properties as well as the asymptotic behaviour of this function for large values of the energy parameter ε.

The single-particle Green function $G(\mathbf{r}t, \mathbf{r}'t')$ is defined as follows (Fetter and Walecka 1971, pp. 64 and 65)

$$G(\mathbf{r}t, \mathbf{r}'t') := -i \langle \Psi_{N,0} | \mathcal{T} \{ \widehat{\psi}_H(\mathbf{r}t) \widehat{\psi}_H^\dagger(\mathbf{r}'t') \} | \Psi_{N,0} \rangle . \tag{8}$$

Here $|\Psi_{N,0}\rangle$ (short for $|\Psi_{N,0}\rangle_H$) stands for the *normalised* (to unity) N-electron *ground state* of $\widehat{H}$ in the Heisenberg representation, and $\mathcal{T}$ for the *fermionic* time-ordering operator. The field operators with subscript H are the Heisenberg representations of the field operators in Sec. 3. Due to the time-ordering operator, the single-particle GF has a finite discontinuity at $t = t'$ (see Appendix B). For the time-Fourier transform of $G(\mathbf{r}t, \mathbf{r}'t')$, which is a function of $t - t'$, we have

$$G(\mathbf{r}, \mathbf{r}; \varepsilon) := \int_{-\infty}^{\infty} dt\, e^{i\varepsilon t/\hbar} G(\mathbf{r}t, \mathbf{r}'0) \equiv G^h(\mathbf{r}, \mathbf{r}'; \varepsilon) + G^p(\mathbf{r}, \mathbf{r}'; \varepsilon) , \tag{9}$$

where the "particle" (G^p) and the "hole" (G^h) part of G are defined as follows (Thouless 1972, pp. 84–89)[15]

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[15] In this reference, the terms "advanced" and "retarded" have been used for what we have called "particle" and "hole", respectively. Our choice is effected by the fact that commonly (see, e.g., Fetter and Walecka 1971, pp. 77–79) "advanced" and "retarded" parts of the GF are defined differently.

$$G^h(\mathbf{r},\mathbf{r}';\varepsilon) := \int_{-\infty}^{0} dt\, \mathrm{e}^{i\varepsilon t/\hbar} G(\mathbf{r}t,\mathbf{r}'0)\,;\;\; G^p(\mathbf{r},\mathbf{r}';\varepsilon) := \int_{0}^{\infty} dt\, \mathrm{e}^{i\varepsilon t/\hbar} G(\mathbf{r}t,\mathbf{r}'0)\,. \tag{10}$$

From now onwards we shall employ operator notation alongside the coordinate and wave-vector (momentum) representations (see Appendix A). It can be shown (Titchmarsh 1939, p. 99) that $\widetilde{G}^h(z)$ ($\widetilde{G}^p(z)$) is analytic in the lower (upper) part of the complex z-plane. Here $\widetilde{G}^h(z)$ and $\widetilde{G}^p(z)$ are obtained by replacing ε (which is supposed to be real-valued) in Eq. (10) by the complex-valued variable z; for $\widetilde{G}^h(z)$ it must hold $\mathrm{Im}(z) < 0$ and for $\widetilde{G}^p(z)$, $\mathrm{Im}(z) > 0$ (for some subtle aspects concerning this *direct* substitution of z for ε in the Fourier-integral representations, see Subsec. 4.8). The correctness of this procedure can be verified by demonstrating that for $z \to \varepsilon$, $G^h(\varepsilon)$ and $G^p(\varepsilon)$ are (uniformly) recovered from $G^h(z)$ and $G^p(z)$, respectively (see Subsec. 2.2).

4.1. *The Lehmann representation for $G(\varepsilon)$*

Here we consider a well-known representation for $G(\varepsilon)$, the Lehmann (1954) representation (Fetter and Walecka 1971, pp. 72–79), which is particularly useful for its exposition of the physical relevance of $G(\varepsilon)$. It also helps us to construct the analytic continuation of $G(\varepsilon)$ into the physical RS. This representation follows through writing down the states and operators in Eq. (8) in terms of their Schrödinger-picture counterparts and making use of the completeness relation for the simultaneous eigenstates of $\widehat{H}$ and the number operator $\widehat{N}$ in the Fock space, i.e. $\sum_{M,s} |\Psi_{M,s}\rangle\langle\Psi_{M,s}| = I$, where $M = 0, 1, \ldots$ denotes the number of electrons and s the remaining quantum numbers that specify an eigenstate of $\widehat{H}$, with $s = 0$ symbolically denoting the GS. This representation reads as follows:

$$G(\mathbf{r},\mathbf{r}';\varepsilon) = \hbar \sum_s f_s(\mathbf{r}) f_s^*(\mathbf{r}') \left\{ \frac{\theta(\mu - \varepsilon_s)}{\varepsilon - \varepsilon_s - i\eta} + \frac{\theta(\varepsilon_s - \mu)}{\varepsilon - \varepsilon_s + i\eta} \right\}, \quad (\eta \downarrow 0), \tag{11}$$

where

$$f_s(\mathbf{r}) := \begin{cases} \langle \Psi_{N-1,s} | \widehat{\psi}(\mathbf{r}) | \Psi_{N,0} \rangle\,, & \text{when } \varepsilon_s < \mu\,, \\ \langle \Psi_{N,0} | \widehat{\psi}(\mathbf{r}) | \Psi_{N+1,s} \rangle\,, & \text{when } \varepsilon_s > \mu\,, \end{cases} \tag{12}$$

a “Lehmann amplitude”, and

$$\varepsilon_s := \begin{cases} E_{N,0} - E_{N-1,s}\,, & \text{when } \varepsilon_s < \mu\,, \\ E_{N+1,s} - E_{N,0}\,, & \text{when } \varepsilon_s > \mu\,; \end{cases} \tag{13}$$

$E_{M,s}$ denotes the eigenenergy corresponding to $|\Psi_{M,s}\rangle$ and μ the "chemical potential" (see Subsec. 4.2). The first term on the right-band side (RHS) of Eq. (11) corresponds to $G^h(\varepsilon)$ and the second to $G^p(\varepsilon)$; the designations "hole part" and "particle part" are seen to indicate the "backward" and "forward" propagations of the *particles* in time, respectively. Mathematically, the positive infinitesimally small "energy" $\pm i\eta$ has its root in the Fourier representations for $\theta(t-t')$ and $\theta(t'-t)$; we have $\theta(\tau) = \pm i\hbar \int_{-\infty}^{\infty} d\varepsilon/(2\pi\hbar) \exp(\mp i\varepsilon\tau/\hbar)/(\varepsilon \pm i\eta)$. For macroscopic and open systems, the summation over s in Eq. (11) involves integrals corresponding to the continuous part of the single-particle spectrum (see Subsec. 2.4).

4.2. *On the "chemical potential"* μ

The "chemical potential" μ in the above expressions should be viewed in the light of the following considerations. For the cases corresponding to $\varepsilon_s < \mu$, from Eq. (13) we have: $\varepsilon_s = \mu_N - \bar{\varepsilon}_s$, where $\mu_N := E_{N,0} - E_{N-1,0}$ and $\bar{\varepsilon}_s := E_{N-1,s} - E_{N-1,0} \geq 0$, from which it follows that $\varepsilon_s \leq \mu_N$. For the cases corresponding to $\varepsilon_s > \mu$ we have: $\varepsilon_s := \mu_{N+1} + \bar{\varepsilon}_s$, where $\mu_{N+1} := E_{N+1,0} - E_{N,0}$ and $\bar{\varepsilon}_s := E_{N+1,s} - E_{N+1,0} \geq 0$, implying $\varepsilon_s \geq \mu_{N+1}$. We observe that introduction of μ is justified only if $\mu_N \leq \mu_{N+1}$, so that $\mu_N \leq \mu \leq \mu_{N+1}$ can apply. Here we shall provide this justification; in fact, as we shall see, we have even $\mu_N < \mu_{N+1}$.

In anticipation of what follows, let $\varepsilon_g := \mu_{N+1} - \mu_N$, which can be rewritten as

$$\varepsilon_g = (E_{N+1,0} - E_{N,0}) - (E_{N,0} - E_{N-1,0}) . \qquad (14)$$

Since the *electronic* many-body states, $\{|\Psi_{M,s}\rangle\}$, that we consider here correspond to one and the same ionic or background external potential, for $M \neq N$ these are *not* charge neutral; for $M > N (M < N)$ they correspond to negatively- (positively-) charged systems. The non-negativeness of ε_g, therefore, amounts to the statement that it is energetically *at least* as costly to add one electron to a charge-neutral system as is to a singly positively-charged system (below we shall show that it is in fact more costly, albeit even by an infinitesimal amount, to do so). In atomic and molecular physics $-\mu_N$ is referred to as the *first ionisation potential* (denoted by $I(Z)$ where Z denotes the atomic number, or number of the protons in the system — for charge neutral systems $Z = N$), and $-\mu_{N+1}$ as the *electron affinity* (denoted by $A(Z)$), so that $\varepsilon_g \equiv I(Z) - A(Z)$; see, e.g., Perdew, Parr, Levy and Balduz (1982). Iu the solid-state physics μ_{N+1} is the lowest (quasi-particle) conduction-band energy (denoted by ε_c) and μ_N the highest (quasi-particle) valence-band energy (denoted by ε_v), so that $\varepsilon_g \equiv \varepsilon_c - \varepsilon_v$; see, e.g., Sham and Schlüter (1985). Hence, introduction of a single constant, μ, in Eq. (11) is justified. For a system in the thermodynamic limit and without gap in its low-lying single-particle-excitation spectrum, μ_{N+1} is *the* chemical potential and further $\mu_{N+1} = \mu_N + \mathcal{O}(N^{-p})$, where $p > 0$.[16] It is interesting to point out that the largest electron affinity and the smallest first ionisation potential in nature amount to 3.62 eV (pertaining to element Cl) and 3.89 eV (pertaining to element Cs), respectively — see, e.g., Dreizler and Gross (1990), p. 24. This implies that as far as the elements in the periodic table are concerned, $\min\{I(Z) - A(Z)\} \gtrsim 0.27$ eV. As for systems in the thermodynamic limit (say, periodic crystals), if $\mu_{N+1} < \mu_N$, from the Lehmann representation in Eq. (11) it would follow that $G(\varepsilon)$ were ill-defined, as in such a case $\widetilde{G}(\varepsilon)$ would possess a continuous set of so-called

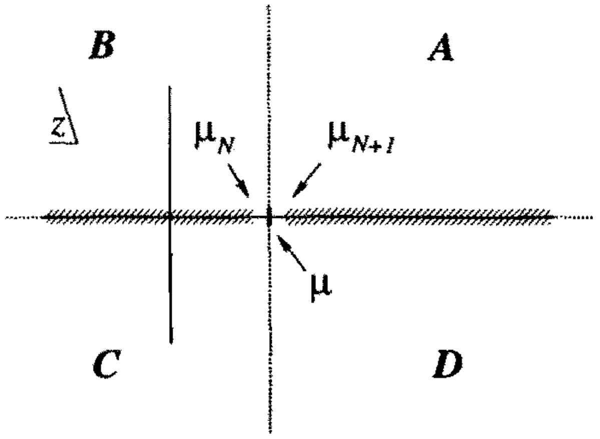

Fig. 3. The complex z-plane and the locations of μ_N, μ and μ_{N+1}, satisfying $\mu_N < \mu < \mu_{N+1}$. Although in the thermodynamic limit μ_N and μ_{N+1} are infinitesimally close for metallic systems ($\mu_N = \mu_{N+1} + \mathcal{O}(N^{-p})$, with $p > 0$), nonetheless the open interval (μ_N, μ_{N+1}) remains non-vanishing. In the interior of this interval $\widetilde{G}(z)$ and $\widetilde{\Sigma}(z)$ are analytic (see Subsecs. 4.5 and 5.1). For systems with a fundamental gap in their quasi-particle (QP) spectrum, $\mu_{N+1} - \mu_N$ is finite and (at the absolute zero of temperature) μ can take on any value within (μ_N, μ_{N+1}). For semiconductors and insulators μ_N coincides with the energy of the top of the valence band and μ_{N+1} with that of the bottom of the conduction band; thus $\mu_{N+1} - \mu_N$ amounts to the QP gap. For finite systems, such as atoms and molecules, $-\mu_N$ coincides with the *first ionisation potential* and $-\mu_{N+1}$ with the *electron affinity*. Following our convention concerning the time-energy Fourier transforms, a *physical* function (say, $f(\varepsilon)$) is obtained from its analytic continuation on the physical Riemann sheet $A \cup B \cup C \cup D$ (i.e. $\widetilde{f}(z)$) through approaching the real energy axis from quadrants A and C.

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[16] The value $p = 1$ as given in Fetter and Walecka (1971), p. 75, is incorrect.

"pinch" singularities for $\varepsilon \in (\mu_{N+1}, \mu_N)$. As the name indicates, "pinch singularities" (Itzykson and Zuber 1985, pp. 302, 303)[17] would "pinch" the contour along which $G(\varepsilon)$ has been defined, so that in transforming $G(\varepsilon)$ to the time domain [for obtaining $G(t)$] one would encounter a non-integrable function; non-pinch singularities, contrary to pinch singularities, can be avoided through deformation of the contour of integration. The condition $\mu_N = \mu_{N+1}$, or $\varepsilon_g = 0$, also corresponds to a pinch singularity in the integral representation for $G(t)$ in terms of $G(\varepsilon)$. We therefore conclude that in all cases it must hold $\mu_N < \mu_{N+1}$, so that (μ_N, μ_{N+1}) is always a finite (even though infinitesimally small) open interval. See Fig. 3.

4.3. *Sums involving the Lehmann amplitudes and energies*

The sets $\{|\Psi_{N-1,s}\rangle | \forall s\}$, $\{|\Psi_{N+1,s}\rangle | \forall s\}$ are *not* complete in the Fock space. They are, however, complete in the subspaces corresponding to, respectively, $N-1$- and $N+1$-electron states. Thus whereas $\sum_s |\Psi_{N\pm1,s}\rangle\langle\Psi_{N\pm1,s}| \neq I$, in such expressions as $\sum_s \langle\Psi_{N,0}|\widehat{\psi}^\dagger(\mathbf{r}')|\Psi_{N-1,s}\rangle\langle\Psi_{N-1,s}|\widehat{\psi}(\mathbf{r})|\Psi_{N,0}\rangle$ and $\sum_s \langle\Psi_{N,0}|\widehat{\psi}(\mathbf{r})|\Psi_{N+1,s}\rangle\langle\Psi_{N+1,s}|\widehat{\psi}^\dagger(\mathbf{r}')|\Psi_{N,0}\rangle$, the completeness relation can be applied. Whence the following two results

$$\begin{aligned}
\sum_s f_s(\mathbf{r}) f_s^*(\mathbf{r}') &\equiv \sum_s \theta(\mu - \varepsilon_s) f_s(\mathbf{r}) f_s^*(\mathbf{r}') + \sum_s \theta(\varepsilon_s - \mu) f_s(\mathbf{r}) f_s^*(\mathbf{r}') \\
&\equiv \sum_s \langle\Psi_{N,0}|\widehat{\psi}^\dagger(\mathbf{r}')|\Psi_{N-1,s}\rangle\langle\Psi_{N-1,s}|\widehat{\psi}(\mathbf{r})|\Psi_{N,0}\rangle \\
&\quad + \sum_s \langle\Psi_{N,0}|\widehat{\psi}(\mathbf{r})|\Psi_{N+1,s}\rangle\langle\Psi_{N+1,s}|\widehat{\psi}^\dagger(\mathbf{r}')|\Psi_{N,0}\rangle \\
&\equiv \langle\Psi_{N,0}|\widehat{\psi}^\dagger(\mathbf{r}')\widehat{\psi}(\mathbf{r}) + \widehat{\psi}(\mathbf{r})\widehat{\psi}^\dagger(\mathbf{r}')|\Psi_{N,0}\rangle \equiv \delta(\mathbf{r}' - \mathbf{r}) , \qquad (15)
\end{aligned}$$

$$\begin{aligned}
\sum_s \theta(\mu - \varepsilon_s) f_s(\mathbf{r}) f_s^*(\mathbf{r}') &\equiv \sum_s \langle\Psi_{N,0}|\widehat{\psi}^\dagger(\mathbf{r}')|\Psi_{N-1,s}\rangle\langle\Psi_{N-1,s}|\widehat{\psi}(\mathbf{r})|\Psi_{N,0}\rangle \\
&\equiv \langle\Psi_{N,0}|\widehat{\psi}^\dagger(\mathbf{r}')\widehat{\psi}(\mathbf{r})|\Psi_{N,0}\rangle =: \frac{1}{2}\rho(\mathbf{r}', \mathbf{r}) \\
&\equiv -iG(\mathbf{r}t, \mathbf{r}'t^+) . \qquad (16)
\end{aligned}$$

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[17] In, e.g., $\int_{-1}^{+1} dx/(x^2 + \eta^2)$, $x = 0$ becomes a "pinch" singularity for $\eta = 0$.

Here $\rho(\mathbf{r}', \mathbf{r})$ stands for the one-particle reduced density matrix; the pre-factor $\frac{1}{2}$ originates from the fact that the index s does *not* involve the spin-coordinate of the electrons; including this, which amounts to an additional trace over the *two* spin states of the electrons, removes this pre-factor. The last result in Eq. (15) follows from the anti-commutation relation for the field operators, and is the statement of the *completeness* of the set of Lehmann amplitudes. This completeness can be expressed as $\sum_s f_s f_s^\dagger = I$, where I stands for the unit operator in the space of one-point functions, with $f_s(\mathbf{r}) = \langle \mathbf{r}|f_s$, and consequently $f_s^*(\mathbf{r}) = f_s^\dagger|\mathbf{r}\rangle$. We note, however, that in general $f_s^\dagger f_{s'} \neq \delta_{s,s'}$; for diminishing values of the coupling constant of the electron-electron interaction, $f_s^\dagger f_{s'} \to \delta_{s,s'}$, when $\varepsilon_s \neq \varepsilon_{s'}$, and the limit is exactly achieved when this coupling constant is identically vanishing.

Making use of the definitions for the Lehmann amplitudes and energies (see Eqs. (12) and (13)), it can easily be shown that

$$\begin{aligned}\Xi_<(\mathbf{r}, \mathbf{r}') &:= \sum_s \theta(\mu - \varepsilon_s)\varepsilon_s f_s(\mathbf{r}) f_s^*(\mathbf{r}') \\ &= \langle \Psi_{N,0}|\widehat{\psi}^\dagger(\mathbf{r}')[\widehat{H}, \widehat{\psi}(\mathbf{r})]_-|\Psi_{N,0}\rangle,\end{aligned} \tag{17}$$

$$\begin{aligned}\Xi_>(\mathbf{r}, \mathbf{r}') &:= \sum_s \theta(\varepsilon_s - \mu)\varepsilon_s f_s(\mathbf{r}) f_s^*(\mathbf{r}') \\ &= \langle \Psi_{N,0}| \left[\widehat{H}, \widehat{\psi}(\mathbf{r})\right]_- \widehat{\psi}^\dagger(\mathbf{r}')|\Psi_{N,0}\rangle\,.\end{aligned} \tag{18}$$

Using the anti-commutation relations for the field operators, the following are readily obtained

$$\begin{aligned}[\widehat{T}, \widehat{\psi}(\mathbf{r})]_- &= -\left[\frac{-\hbar^2}{2m_e}\nabla^2\right]\widehat{\psi}(\mathbf{r})\,, \\ [\widehat{U}_v, \widehat{\psi}(\mathbf{r})]_- &= -v(\mathbf{r})\widehat{\psi}(\mathbf{r})\,, \\ [\widehat{U}_w, \widehat{\psi}(\mathbf{r})]_- &= -\int d^3r''\, w(\mathbf{r}, \mathbf{r}'')\widehat{\psi}(\mathbf{r}'')\,, \\ [\widehat{V}, \widehat{\psi}(\mathbf{r})]_- &= -\int d^3r''\, v_c(\mathbf{r} - \mathbf{r}'')\widehat{\psi}^\dagger(\mathbf{r}'')\widehat{\psi}(\mathbf{r}'')\widehat{\psi}(\mathbf{r})\,.\end{aligned} \tag{19}$$

Thus,

$$\Xi_<(\mathbf{r},\mathbf{r}') = \frac{1}{2}\left\{\left[\frac{-\hbar^2}{2m_e}\nabla^2 + v(\mathbf{r})\right]\rho(\mathbf{r},\mathbf{r}') + \int d^3r''w(\mathbf{r},\mathbf{r}'')\rho(\mathbf{r}'',\mathbf{r}')\right\}$$
$$+ \int d^3r''v_c(\mathbf{r}-\mathbf{r}'')\langle\Psi_{N,0}|\widehat{\psi}^\dagger(\mathbf{r}')\widehat{\psi}^\dagger(\mathbf{r}'')\widehat{\psi}(\mathbf{r}'')\widehat{\psi}(\mathbf{r})|\Psi_{N,0}\rangle\,, \qquad (20)$$

$$\Xi_>(\mathbf{r},\mathbf{r}') = \left[\frac{-\hbar^2}{2m_e}\nabla^2 + v(\mathbf{r})\right]\delta(\mathbf{r}-\mathbf{r}') + w(\mathbf{r},\mathbf{r}')$$
$$- \frac{1}{2}\left\{\left[\frac{-\hbar^2}{2m_e}\nabla^2 + v(\mathbf{r})\right]\rho(\mathbf{r},\mathbf{r}') + \int d^3r''w(\mathbf{r},\mathbf{r}'')\rho(\mathbf{r}'',\mathbf{r}')\right\}$$
$$+ \int d^3r''v_c(\mathbf{r}-\mathbf{r}'')\langle\Psi_{N,0}|\widehat{\psi}^\dagger(\mathbf{r}'')\widehat{\psi}(\mathbf{r}'')\widehat{\psi}(\mathbf{r})\widehat{\psi}^\dagger(\mathbf{r}')|\Psi_{N,0}\rangle\,. \qquad (21)$$

The two terms involving v_c in the above expressions *cannot* be explicitly expressed in terms of such GS quantities as n or ρ. However, a simple decoupling approximation yields[18]

$$\int d^3r''v_c(\mathbf{r}-\mathbf{r}'')\langle\Psi_{N,0}|\widehat{\psi}^\dagger(\mathbf{r}')\widehat{\psi}^\dagger(\mathbf{r}'')\widehat{\psi}(\mathbf{r}'')\widehat{\psi}(\mathbf{r})|\Psi_{N,0}\rangle$$
$$\begin{cases} = \dfrac{N(N-1)}{2}\int d^3r''v_c(\mathbf{r}-\mathbf{r}'')g(\mathbf{r},\mathbf{r}'') \approx \dfrac{1}{2}v_H(\mathbf{r};[n])n(\mathbf{r})\,, & \text{when } \mathbf{r}=\mathbf{r}'\,, \\ \approx \dfrac{1}{2}(v_H(\mathbf{r};[n]) - v_c(\mathbf{r}-\mathbf{r}'))\rho(\mathbf{r}',\mathbf{r})\,, & \text{when } \mathbf{r}\neq\mathbf{r}'\,, \end{cases} \qquad (22)$$

$$\int d^3r''v_c(\mathbf{r}-\mathbf{r}'')\langle\Psi_{N,0}|\widehat{\psi}^\dagger(\mathbf{r}'')\widehat{\psi}(\mathbf{r}'')\widehat{\psi}(\mathbf{r})\widehat{\psi}^\dagger(\mathbf{r}')|\Psi_{N,0}\rangle$$
$$\approx v_H(\mathbf{r};[n])\left(\delta(\mathbf{r}-\mathbf{r}') - \frac{1}{2}\rho(\mathbf{r}',\mathbf{r})\right)\,, \qquad (23)$$

where

$$v_H(\mathbf{r};[n]) := \int d^3r''v_c(\mathbf{r}-\mathbf{r}'')n(\mathbf{r}'') \qquad (24)$$

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[18] In Eq. (22) the distinction between the cases corresponding to $\mathbf{r}=\mathbf{r}'$ and $\mathbf{r}\neq\mathbf{r}'$ arises from the process of *normal ordering* (Wick 1950, Klein and Prange 1958) which for simplicity we have not systematically taken care of in the present work (thus, for instance, rather than working with $\widehat{H}$, we must have been working with $:\widehat{H}:$). For the case of $\mathbf{r}=\mathbf{r}'$ we have explicitly enforced the normal ordering.

stands for the Hartree potential and $g(\mathbf{r}, \mathbf{r}'')$ for the (van Hove) pair-correlation function presented in Eq. (154) below. We shall see in Subsec. 4.6 that although the RHS of Eqs. (22) and (23) are approximate, their sum, i.e. $v_H(\mathbf{r}; [n])\delta(\mathbf{r} - \mathbf{r}') - \frac{1}{2}v_c(\mathbf{r} - \mathbf{r}')\ \rho(\mathbf{r}', \mathbf{r})$, *is* the exact result for the sum of their left-hand sides (LHSs). We have to point out that in arriving at Eqs. (22) and (23) we have multiplied the contributions leading to $v_H(\mathbf{r}; [n])$ by a factor of two. This factor accounts for a trace over an *internal* spin degree of freedom; if we had adopted the notation in which the electron field operators are furnished with spin index, then such an *ad hoc* introduction of this factor were not needed.

4.4. *A symmetry property of G*

Here we demonstrate a symmetry property of $G(\mathbf{r}, \mathbf{r}'; \varepsilon)$; in the process of this demonstration, we encounter a number of important issues that are closely tied with the time-inversion symmetry of the GS of the system under consideration. To this end let $\widehat{\mathbf{Q}}_\alpha := \exp(i\alpha\delta\mathbf{r} \cdot \widehat{\mathbf{p}}/\hbar)$, where $\delta\mathbf{r} := \mathbf{r}' - \mathbf{r}$ and $\widehat{\mathbf{p}}$ stands for the one-particle momentum operator (see Appendix A). Thus $\widehat{\mathbf{Q}}_\alpha$ is the translation operator, transforming functions of $\mathbf{r}$, along $\delta\mathbf{r}$, to those of $\mathbf{r}'$ when α is increased from 0 to 1. We have $f_s(\mathbf{r}') = \widehat{\mathbf{Q}}_1 f_s(\mathbf{r})$. We define now $A_{s;\alpha} := f_s(\mathbf{r})[\widehat{\mathbf{Q}}_\alpha f_s^*(\mathbf{r})] - [\widehat{\mathbf{Q}}_\alpha f_s(\mathbf{r})]f_s^*(\mathbf{r})$, which for $\alpha = 1$ measures the amount by which $f_s(\mathbf{r})f_s^*(\mathbf{r}')$ differs from $f_s(\mathbf{r}')f_s^*(\mathbf{r})$. Obviously $A_{s;0} \equiv 0$. By some straightforward algebra it can be shown that for $n > 1$, $\partial^n A_{s;\alpha}/\partial\alpha^n|_{\alpha=0} = (i\delta\mathbf{r} \cdot \widehat{\mathbf{p}}/\hbar)^{n-1}\partial A_{s;\alpha}/\partial\alpha|_{\alpha=0}$. Thus, if $\partial A_{s;\alpha}/\partial\alpha|_{\alpha=0} \equiv 0$, it follows that $A_{s;\alpha} \equiv 0$, so that $f_s(\mathbf{r})f_s^*(\mathbf{r}') = f_s(\mathbf{r}')f_s^*(\mathbf{r})$. It can easily be verified that $\partial A_{s;\alpha}/\partial\alpha|_{\alpha=0} = -2im_e\hbar^{-1}\delta\mathbf{r} \cdot \mathbf{j}_{p;s}(\mathbf{r})$, where $\mathbf{j}_{p;s}(\mathbf{r})$ stands for the *paramagnetic* particle flux density[19] corresponding to the Lehmann amplitude $f_s(\mathbf{r})$. The total paramagnetic particle flux density corresponding to the GS of the interacting system under consideration is equal to $\mathbf{j}_p(\mathbf{r}) = \sum_s \theta(\mu - \varepsilon_s)\mathbf{j}_{p;s}(\mathbf{r})$. This flux density is *not* gauge invariant.

The gauge-invariant, or physical, particle flux density in the GS of the N-electron system, i.e. $\mathbf{j}(\mathbf{r}) := e^{-1}\delta E_{N,0}/\delta\mathbf{A}(\mathbf{r})$, in general consists of *three* contributions (Landau and Lifshitz 1977, pp. 472 and 473): one is proportional to the gradient of the difference of densities of electrons corresponding to different spins (Zeeman contribution), one is proportional to the product of the total charge density and the external vector potential $\mathbf{A}$, and the last is the above-mentioned paramagnetic particle flux density $\mathbf{j}_p(\mathbf{r})$. In general, for

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[19] The paramagnetic *current* density is $-e\mathbf{j}_{p;s}(\mathbf{r})$, with $-e < 0$ the electron charge.

spin-compensated systems the first contribution is identically vanishing. Since, however, $\widehat{H}$ in the present work does not involve the Zeeman term, this contribution is in our case vanishing by construction. In the Coulomb or transverse gauge[20] $\boldsymbol{\nabla} \cdot \mathbf{A} = 0$ (Mahan 1981, p. 62), *and* in the absence of an external magnetic field, the second contribution is also vanishing. When the GS possesses time-reversal symmetry (in absence of external magnetic field), the *physical* particle flux density is identically vanishing, so that in the present case where the first two contributions to the physical particle flux density are vanishing, it must hold that $\mathbf{j}_p(\mathbf{r}) \equiv \mathbf{0}$. Now the time-reversal symmetry implies that to each elementary "current" $\mathbf{j}_{p;s}(\mathbf{r})$ must correspond a counter current, the time-reversed current, $\mathbf{j}_{p;\bar{s}}(\mathbf{r}) = -\mathbf{j}_{p;s}(\mathbf{r})$ [call this, property (a)] with $\varepsilon_{\bar{s}} = \varepsilon_s$ [call this, property (b)]. This degeneracy, whose occurrence embodies Kramers' theorem (Landau and Lifshitz 1977, pp. 223–226, Callaway 1964, pp. 52–54),[21] maintains the thermodynamic balance between "currents" and "time-reversed currents". From property (a) we have $f_{\bar{s}}(\mathbf{r}) \equiv e^{i\theta_s} f_s^*(\mathbf{r})$, with θ_s real and independent of $\mathbf{r}$, so that $B_s(\mathbf{r},\mathbf{r}') := f_s(\mathbf{r}) f_s^*(\mathbf{r}') + f_{\bar{s}}(\mathbf{r}) f_{\bar{s}}^*(\mathbf{r}')$ is a real-valued symmetric function of $\mathbf{r}$ and $\mathbf{r}'$. Let now $F(x)$ be an arbitrary function. From properties (a) and (b) it follows that not only $\mathbf{j}_p(\mathbf{r}) = \mathbf{0}$, but also that $\sum_s F(\varepsilon_s) f_s(\mathbf{r}) f_s^*(\mathbf{r}') \equiv {\sum'}_s F(\varepsilon_s) B_s(\mathbf{r},\mathbf{r}')$ is a symmetric function of $\mathbf{r}$ and $\mathbf{r}'$; here ${\sum'}_s$ denotes a summation involving either s *or* its time-reversed counterpart $\bar{s}$, but *not* both. In particular we have (the $F(\varepsilon_s)$ involved here is the term enclosed by the curly brackets on the RHS of Eq. (11))

$$G(\mathbf{r},\mathbf{r}';\varepsilon) \equiv G(\mathbf{r}',\mathbf{r};\varepsilon)\,. \tag{25}$$

From the same line of reasoning leading to Eq. (25), one further obtains (see Eq. (16))

$$\rho(\mathbf{r},\mathbf{r}') = \rho(\mathbf{r}',\mathbf{r})\,. \tag{26}$$

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[20] The instantaneous nature of the Hartree potential $v_H(\mathbf{r};[n])$ follows this choice for the gauge. See Footnote 14.

[21] Kramers' theorem guarantees degeneracy of the energy levels for cases where the spinors, *or* the irreducible representations of the symmetry group of the Schrödinger equation, are essentially complex. This applies specifically to systems with *odd* number of electrons (which are spin-1/2 particles) and generally to those in which the sum of spins of the constituent particles is half-integer. For systems of spin-less fermions in the thermodynamic limit, subjected to the box- or the periodic-boundary condition, Kramers' theorem applies exclusively on account of the irreducible representations of the translation group (whether discrete or continuous) being essentially complex. For a detailed discussion of the significance of the time-reversal symmetry in solids see Cornwell (1969), Ch. 5, Sec. 7.

For illustration of the above details, consider a non-interacting uniform-electron system enclosed in a macroscopic box of volume Ω. For this system we have (see Appendix A) $f_s(\mathbf{r}) \leftrightarrow f_{\mathbf{k}}(\mathbf{r}) := \exp(i\mathbf{k}\cdot\mathbf{r})/\Omega^{1/2}$, $\varepsilon_s \leftrightarrow \varepsilon^0_{\mathbf{k}} := \hbar^2 k^2/(2m_e)$, for both $\varepsilon^0_{\mathbf{k}} < \mu^0$ and $\varepsilon^0_{\mathbf{k}} > \mu^0$ where $\mu^0 := \hbar^2 k_F^2/(2m_e)$ with k_F the Fermi wave-number; $\sum_s(\ldots) \leftrightarrow (\Omega/[2\pi]^3)\int d^3k(\ldots)$. With $s \leftrightarrow \mathbf{k}$, we can identify $\bar{s}$ with $-\mathbf{k}$: we have both $\varepsilon^0_{-\mathbf{k}} = \varepsilon^0_{\mathbf{k}}$ and $f_{-\mathbf{k}}(\mathbf{r}) = f^*_{\mathbf{k}}(\mathbf{r})$. With reference to our above considerations, the latter equality is in general only satisfied up to a phase factor: at different $\mathbf{k}$-points, the wavefunctions can be solved under different gauge conditions. By considering the momentum $\mathbf{p} \equiv \hbar\mathbf{k}$ as a dynamical variable, we observe that $-\mathbf{k} \leftrightarrow \bar{s}$ indeed corresponds to the "time-reversed" state associated with $\mathbf{k} \leftrightarrow s$.

4.5. *Analytic continuation of $G(\varepsilon)$, $\widetilde{G}(z)$*

We now *define* the following function[22]

$$\widetilde{G}(\mathbf{r},\mathbf{r}';z) := \hbar \sum_s \frac{f_s(\mathbf{r}) f_s^*(\mathbf{r}')}{z - \varepsilon_s}\,. \tag{27}$$

This function has the property

$$\lim_{\eta\downarrow 0} \widetilde{G}(\varepsilon \pm i\eta) \equiv G(\varepsilon)\,, \quad \text{when } \varepsilon \gtrless \mu\,. \tag{28}$$

Hence $\widetilde{G}(z)$ in Eq. (27) is the analytic continuation of $G(\varepsilon)$, as represented in Eq. (11), into the physical RS of the complex z-plane (Subsecs. 2.2 and 2.4). One can in all calculations involving G, replace this by $\widetilde{G}$ provided that on taking the limit $\mathrm{Im}(z) \to 0$, $\mathrm{Re}(z-\mu) \times \mathrm{Im}(z) > 0$ is satisfied. For instance, in transforming $G(\varepsilon)$ to the time domain, the integral along the ε-axis of $G(\varepsilon)$ can be replaced by one along a contour C in the complex z-plane of $\widetilde{G}(z)$, on the condition that on each point along C, $\mathrm{Re}(z-\mu) \times \mathrm{Im}(z) > 0$ is obeyed (see Fig. 4); since singularities of $\widetilde{G}(z)$ are all along the real axis (see Eq. (27) — Luttinger 1961), it is *not* necessary that along C, $\mathrm{Im}(z) \to 0$.

From Eqs. (27) and (25) it follows that (see Luttinger 1961)

$$\widetilde{G}(\mathbf{r},\mathbf{r}';z^*) = \widetilde{G}^*(\mathbf{r},\mathbf{r}';z)\,, \tag{29}$$

i.e. $\widetilde{G}(z)$ possesses reflection symmetry with respect to the real energy axis. In the theory of functions of complex variables, functions which are analytic

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[22] $\widetilde{G}(z) = \hbar\sum_s f_s f_s^\dagger/(z-\varepsilon_s)$; see text following Eq. (16) above.

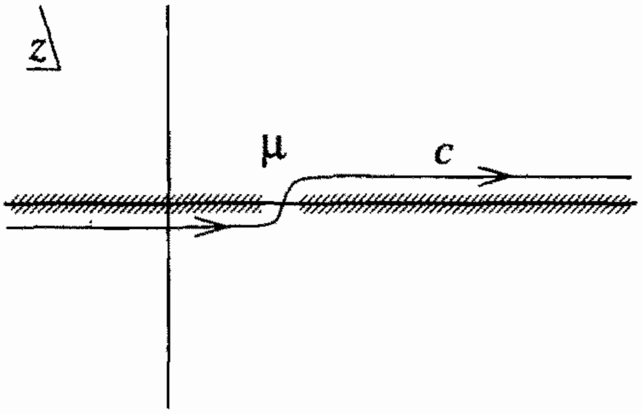

Fig. 4. The Contour of integration on the physical Riemann sheet of the complex z-plane. When the imaginary parts of the points on this contour are made to approach zero, a function such as $\widetilde{f}(z)$ on C approaches the *physical* function $f(\varepsilon)$. Recall that $f(\varepsilon) \equiv \lim_{\eta\downarrow 0} \widetilde{f}(\varepsilon \pm i\eta)$, for $\varepsilon > \mu$ and $\varepsilon < \mu$. The shaded sections of the real axis signify branch cuts of $\widetilde{f}(z)$. Examples for $\widetilde{f}(z)$ are $\widetilde{G}(z)$ and $\widetilde{\Sigma}(z)$.

everywhere on the complex plane and are real-valued on some finite interval of the real axis, possess a similar reflection property, Schwarz's reflection property (Titchmarsh 1939, p. 155, Spiegel 1974, p. 266). In the light of this, the reflection property of $\widetilde{G}(z)$ can be understood by the observation that $\widetilde{G}(z)$ is analytic everywhere on the complex z-plane, excluding some points or intervals on the real axis, and is real-valued over the finite, albeit possibly infinitesimally small (in the thermodynamic limit), interval (μ_N, μ_{N+1}) — see Subsec. 4.2.

We define the *physical* spectral function (whence the subscript p) as follows

$$A_p(\mathbf{r}, \mathbf{r}'; \varepsilon) := \mp \frac{1}{2\pi i} \lim_{\eta\downarrow 0} \left\{ \widetilde{G}(\mathbf{r}, \mathbf{r}'; \varepsilon + i\eta) - \widetilde{G}(\mathbf{r}, \mathbf{r}'; \varepsilon - i\eta) \right\}$$

$$\equiv \pm\hbar \sum_s f_s(\mathbf{r}) f_s^*(\mathbf{r}') \delta(\varepsilon - \varepsilon_s)\,, \quad \varepsilon \gtrless \mu\,. \tag{30}$$

This deviates from the commonly-used definition where the upper signs are taken, irrespective of the value of ε; our definition takes account of the change in sign attached to $i\eta$ in the Lehmann representation for $G(\varepsilon)$ as ε is increased from below μ to above μ. The "physical" spectral function satisfies the following zeroth-order sum-rule:

$$\int_{-\infty}^{+\infty} d\varepsilon A_p(\mathbf{r}, \mathbf{r}'; \varepsilon) = \hbar\{\delta(\mathbf{r} - \mathbf{r}') - \rho(\mathbf{r}, \mathbf{r}')\}\,. \tag{31}$$

In the equivalent sum-rule for the standard spectral function, one only encounters $\hbar\delta(\mathbf{r} - \mathbf{r}')$ on the RHS.

4.6. *Large-$|\varepsilon|$ Behaviour of $G(\varepsilon)$*

From the Lehmann representation for $G(\varepsilon)$ it directly follows that

$$G(\varepsilon) \sim \frac{G_{\infty_1}}{\varepsilon} + \frac{G_{\infty_2}}{\varepsilon^2}, \quad \text{for} \quad |\varepsilon| \to \infty, \tag{32}$$

where (see Eqs. (15), (17) and (18))

$$\begin{aligned} G_{\infty_1}(\mathbf{r},\mathbf{r}') &:= \hbar\delta(\mathbf{r}-\mathbf{r}'), \\ G_{\infty_2}(\mathbf{r},\mathbf{r}') &:= \hbar\sum_s \varepsilon_s f_s(\mathbf{r}) f_s^*(\mathbf{r}') =: \hbar(\Xi_<(\mathbf{r},\mathbf{r}') + \Xi_>(\mathbf{r},\mathbf{r}')). \end{aligned} \tag{33}$$

It can easily be shown that

$$G_{\infty_2} \equiv \frac{-1}{\pi}\int_{-\infty}^{+\infty} d\varepsilon\varepsilon\widetilde{G}''(\varepsilon+i\eta), \quad \eta \downarrow 0. \tag{34}$$

Here $\widetilde{G}''(z) := \{\widetilde{G}(z) - \widetilde{G}^\dagger(z)\}/(2i)$. Thus G_{∞_2} is equal to the first energy moment of $\widetilde{G}''(\varepsilon+i\eta)$ which for $\varepsilon < \mu$ is equal to $-G''(\varepsilon)$ and for $\varepsilon > \mu$ equal to $G''(\varepsilon)$.

Introducing Eqs. (20) and (21) into Eq. (33) and some algebra yields

$$\begin{aligned} G_{\infty_2}(\mathbf{r},\mathbf{r}') = \hbar\Bigg\{ & \left[\frac{-\hbar^2}{2m_e}\nabla^2 + v(\mathbf{r}) + v_H(\mathbf{r};[n])\right]\delta(\mathbf{r}-\mathbf{r}') + w(\mathbf{r},\mathbf{r}') \\ & - \frac{1}{2}v_c(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r},\mathbf{r}')\Bigg\}. \end{aligned} \tag{35}$$

The last term in Eq. (35) is nothing but the *non-local* exchange (or Fock) potential which occurs in the Hartree–Fock equation. It must be noted, however, that the ρ here is the *exact* ρ and not that which is calculated within the Hartree–Fock framework (see Subsec. 9.7). Since $v_H(\mathbf{r},[n])$ and $v_c(\mathbf{r}-\mathbf{r}')$ both vanish for the vanishing strength of the electron-electron interaction, from Eq. (35) one directly infers that for the non-interacting counterpart of G_{∞_2}, namely $G_{0;\infty_2}$, it must hold

$$G_{0;\infty_2}(\mathbf{r},\mathbf{r}') = \hbar\left\{\left[\frac{-\hbar^2}{2m_e}\nabla^2 + v(\mathbf{r})\right]\delta(\mathbf{r}-\mathbf{r}') + w(\mathbf{r},\mathbf{r}')\right\}. \tag{36}$$

It is then interesting to realise that

$$\begin{aligned}
&\frac{1}{\hbar^2}\{-G_{0;\infty_2}(\mathbf{r},\mathbf{r}') + G_{\infty_2}(\mathbf{r},\mathbf{r}')\} \\
&\quad = \frac{1}{\hbar} v_H(\mathbf{r};[n])\delta(\mathbf{r}-\mathbf{r}') - \frac{1}{2\hbar} v_c(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r},\mathbf{r}') \\
&\quad \equiv \Sigma^{HF}(\mathbf{r},\mathbf{r}') := \Sigma^{H}(\mathbf{r},\mathbf{r}') + \Sigma^{F}(\mathbf{r},\mathbf{r}'),
\end{aligned} \tag{37}$$

where Σ^{HF} stands for the SE operator within the Hartree–Fock scheme (see Subsecs. 5.1, 6.3 and 9.6), with $\Sigma^{H}(\mathbf{r},\mathbf{r}') := \hbar^{-1} v_H(\mathbf{r};[n])\delta(\mathbf{r}-\mathbf{r}')$ the Hartree SE and $\Sigma^{F}(\mathbf{r},\mathbf{r}') := (-2\hbar)^{-1} v_c(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r},\mathbf{r}')$ the Fock SE. As we have mentioned above, ρ here is the *exact* one-particle reduced density matrix.

4.7. $\widetilde{G}(z)$ *is invertible*

In view of our interest concerning analytic properties of the SE operator in the complex energy plane (Subsec. 5.1), here we inspect whether $\widetilde{G}(z)$ can have any zero(s) in the complex energy plane (since $\widetilde{G}(z)$ is an operator, "zero(s)" here means "zero eigenvalue(s)") — see Luttinger (1961). For $z = \varepsilon' + i\varepsilon''$, with ε' and ε'' ($\varepsilon'' \neq 0$) both real-valued, $\widetilde{G}(z)$ can be written as $\mathcal{G}'(\varepsilon',\varepsilon'') + i\mathcal{G}''(\varepsilon',\varepsilon'')$. This is effected through application of $1/[z-\varepsilon_s] = (\varepsilon'-\varepsilon_s)/[(\varepsilon'-\varepsilon_s)^2 + \varepsilon''^2] - i\varepsilon''/[(\varepsilon'-\varepsilon_s)^2 + \varepsilon''^2]$ in Eq. (27). It follows that $\mathcal{G}''(\varepsilon',\varepsilon'')$ *cannot* have any zero (i.e. zero eigenvalue) for $\varepsilon'' \neq 0$. This is demonstrated as follows: Since (see Footnote 22) with $\alpha_s := -\varepsilon''/[(\varepsilon'-\varepsilon_s)^2 + \varepsilon''^2]$, we have $\mathcal{G}'' = \hbar \sum_s \alpha_s f_s f_s^\dagger$, for an *arbitrary* one-particle state vector $|\beta\rangle$, $\langle\beta|\mathcal{G}''|\beta\rangle = \hbar\sum_s \alpha_s\, |\langle\beta|f_s|^2$ holds. Following the fact that $\{f_s(\mathbf{r})\}$ is a *complete* set (though not orthogonal — see Eq. (15) and text following Eq. (16) above), $|\langle\beta|f_s|^2 > 0$ for *some* s, so that $\alpha_s \neq 0$ for *all* s implies that $\langle\beta|\mathcal{G}''|\beta\rangle \neq 0$. This completes the demonstration that no eigenvalue of $\mathcal{G}''$ can be vanishing for $\varepsilon'' \neq 0$, for if this were not the case, then by choosing $|\beta\rangle$ to be the eigenvector corresponding to the vanishing eigenvalue, the latter inequality would be violated.

Now since $\mathcal{G}''(\varepsilon',\varepsilon'')$ is Hermitian, it has real-valued eigenvalues and our above consideration implies that $\mathcal{G}''(\varepsilon',\varepsilon'')$ is negative (positive) definite for $\varepsilon'' > 0$ ($\varepsilon'' < 0$). Further, since $\mathcal{G}'(\varepsilon',\varepsilon'')$ is also Hermitian, it has similarly real eigenvalues which, however, can be of any sign. Now, owing to the imaginary unit in $\mathcal{G} := \mathcal{G}' + i\mathcal{G}''$, the expectation value of $\mathcal{G}(\varepsilon',\varepsilon'') \equiv \widetilde{G}(z)$, for $\varepsilon'' \neq 0$, with respect to *any* single-particle state (like the above $|\beta\rangle$) has a *non-vanishing* imaginary part, so that the single-particle GF *cannot* possess zero eigenvalues on the physical RS of the complex z-plane, that is $\widetilde{G}(z)$ is invertible for $\mathrm{Im}(z) \neq 0$.

4.8. *Connection between analytic continuation and choice of representation*

It is in place that we pause for a while and consider some specific aspect related to the analytic properties of $\widetilde{G}(z)$, $\widetilde{G}^h(z)$ and $\widetilde{G}^p(z)$. Above we have mentioned that the latter two functions can be obtained through a direct *substitution* of z for ε in their defining expressions in Eq. (10); it is required, however, that in the case of $\widetilde{G}^h(z)$, $\mathrm{Im}(z) < 0$ and in the case of $\widetilde{G}^p(z)$, $\mathrm{Im}(z) > 0$. A substitution of this kind in the defining expression for $G(\varepsilon)$ in Eq. (9) for *any* complex z gives rise to a non-existent (i.e. divergent) integral; in the cases of $\widetilde{G}^h(z)$ and $\widetilde{G}^p(z)$ we encounter the same difficulty for $\mathrm{Im}(z) > 0$ and $\mathrm{Im}(z) < 0$, respectively. Yet in spite of these restrictions, it is readily verified that $\widetilde{G}(z)$ in Eq. (27) is nothing but $G(z)$, that is $\widetilde{G}(z)$ is obtained by *substituting* z for ε, which is real-valued, in the Lehmann representation for $G(\varepsilon)$. Similarly, $\widetilde{G}^h(z)$ and $\widetilde{G}^p(z)$ are obtained by direct substitution of z for ε in their respective expressions determined from the Lehmann representation (see text following Eq. (13) above). In particular, from the expressions for $\widetilde{G}(z)$, $\widetilde{G}^h(z)$ and $\widetilde{G}^p(z)$ as derived from the Lehmann representation for $G(\varepsilon)$, it can readily be deduced that these functions are bounded over the *entire* complex z-plane corresponding to $\mathrm{Im}(z) \neq 0$. A most natural question would be: why in obtaining the analytic continuation for, say, $G(\varepsilon)$ a direct *substitution* of z for ε in one representation for $G(\varepsilon)$ (namely, the Fourier-*integral* representation) is not valid, while in a different representation (namely, the Lehmann representation) such substitution is legitimate? Are not different representations of a function supposed to be equivalent?

The answer to the above questions lies in the fact that while $\exp(izt/\hbar)$ is bounded for *real* values of z (we have $|\exp(izt/\hbar)| = 1$), it is unbounded when: (i) $t \in (-\infty, \infty)$ and $\mathrm{Im}(z) \neq 0$; (ii) $t \in (-\infty, 0)$ and $\mathrm{Im}(z) > 0$; (iii) $t \in (0, \infty)$ and $\mathrm{Im}(z) < 0$. For the Fourier *integral* (*integral* in the sense of a Riemann *sum*) to exist, it is necessary that when $\mathrm{Im}(z) \neq 0$, the function with which $\exp(izt/\hbar)$ is multiplied turns the integrand *absolutely* integrable. Since magnitude of $G(\mathbf{r}t, \mathbf{r}'0)$ does not decrease exponentially, for the existence of the Fourier *integrals*, in the light of (i)–(iii), we are to impose restrictions upon $\mathrm{Im}(z)$. That despite this, *substitution* of z (with $\mathrm{Im}(z) \neq 0$) for ε in the Lehmann representation for $G(\varepsilon)$ yields a bounded result, is to do with the fact that even though for an inappropriately chosen z (i.e., chosen in disregard to (i)–(iii)), the integrand in the Fourier integral is unbounded, the associated Riemann *sum* is nevertheless *conditionally* convergent, or it is *summable*. In Subsec. 2.3 we have considered summation of a manifestly divergent series by means of the Borel transformation. There we have observed the direct association between the divergence of a series and the singularity in the analytic function associated with it. In the present case, the real values of ε at which $\widetilde{G}(z \to \varepsilon)$ is unbounded, are those for which the Riemann sums are truly divergent, i.e. not summable.

An example should clarify the above observations. Consider $\widetilde{g}(z) := (i/\hbar) \cdot \int_0^\infty dt \exp(-i[z - \varepsilon_0]t/\hbar)$, where we assume ε_0 to be real. For $\mathrm{Im}(z) < 0$, the integrand of $\widetilde{g}(z)$ is absolutely integrable and one trivially obtains $\widetilde{g}(z) = 1/(z - \varepsilon_0)$. It is seen that $\widetilde{g}(z)$ is analytic everywhere (even on the half-plane $\mathrm{Im}(z) \geq 0$) except at $z = \varepsilon_0$. Let us now express the t-integral as a Riemann sum: $\widetilde{g}(z) = \lim_{\Delta t \downarrow 0} (i\Delta t/\hbar) \sum_{n=0}^\infty [\widetilde{h}(z)]^n$ where $\widetilde{h}(z) := \exp(-i[z - \varepsilon_0]\Delta t/\hbar)$. The geometric series involved here is uniformly convergent provided $|\widetilde{h}(z)| < 1$; in this case, using some elementary algebra one readily obtains $\widetilde{g}(z) = 1/(z - \varepsilon_0)$, which is exactly the result presented above. On the other hand, since $|\widetilde{h}(z)| > 1$ for $\mathrm{Im}(z) > 0$, we observe that $\mathrm{Im}(z) > 0$ indeed renders the above Riemann sum divergent; as mentioned above, this sum can be evaluated through application of, e.g., the Borel summation technique; not surprisingly[23] one again obtains $\widetilde{g}(z) = 1/(z - \varepsilon_0)$.

We conclude that direct substitution of z for ε in the Fourier-integral representation of a function, such as $G(\varepsilon)$, requires an additional step of resummation of a divergent (asymptotic) series (i.e. a Riemann sum).[24] Branch points of, say, $\widetilde{G}(z)$ are those z points around which $\widetilde{G}(z)$ does not allow for a *uniform* asymptotic Riemann sum (Stokes' phenomenon — see Subsec. 2.3).[25]

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[23] For the reason that $\widetilde{g}(z)$ as obtained for the case $\mathrm{Im}(z) < 0$ is a *regular* function of z so that through the process of analytic continuation, one would immediately deduce that $\widetilde{g}(z) = 1/(z - \varepsilon_0)$ for *all* z.

[24] The set $\{[\widetilde{h}(z)]^n | n = 0, 1 \ldots\}$ in our example is indeed an asymptotic sequence for $\mathrm{Im}(z) < 0$.

[25] The following is worth mentioning (Whittaker and Watson 1927, pp. 98 and 99): There are cases where two infinite series *represent* the same analytic function but are suited for two different, i.e. non-overlapping, regions of the z-plane. There are also cases where one infinite series represents two entirely different analytic functions in two different regions of the z plane. Consider $\sum_{n=0}^\infty z^n$ and $\sum_{n=0}^\infty (-1)^{n+1}(z-2)^n$ both of which *represent* $1/(1-z)$. On the other hand, $(z + 1/z)/2 + \sum_{n=1}^\infty (z - 1/z)(1/[1 + z^n] - 1/[1 + z^{n-1}])$ represents z when $|z| < 1$ and $1/z$ when $|z| > 1$.

5. The (Proper) Self-Energy $\Sigma(\varepsilon)$ and its Analytic Continuation $\widetilde{\Sigma}(z)$

The self-energy operator plays the role of a "scattering potential" through whose action the behaviour of the single-particle Green function of a system of "non-interacting" electrons is modified into that of the fully interacting system. In this Section we deal with this operator and a number of its salient properties.

5.1. *Analyticity of $\widetilde{\Sigma}(z)$ and some consequences*

In Subsec. 4.7 we arrived at the conclusion that for $\mathrm{Im}(z) \neq 0$, $\widetilde{G}(z)$ is invertible, i.e. $\widetilde{G}^{-1}(z)$ is *bounded*. The same holds for $\widetilde{G}_0(z)$, i.e. for $\mathrm{Im}(z) \neq 0$, $\widetilde{G}_0^{-1}(z)$ is bounded. Thus the Dyson equation,

$$\widetilde{G}(z) = \widetilde{G}_0(z) + \widetilde{G}_0(z)\widetilde{\Sigma}(z)\widetilde{G}(z)\,, \tag{38}$$

can be written in the alternative form

$$\widetilde{\Sigma}(z) = \widetilde{G}_0^{-1}(z) - \widetilde{G}^{-1}(z)\,. \tag{39}$$

From Eq. (39) it follows that $\widetilde{\Sigma}(z)$ is bounded for $\mathrm{Im}(z) \neq 0$. Through differentiating both sides of Eq. (38) with respect to z (recall that $\widetilde{G}(z)$ and $\widetilde{G}_0(z)$ are analytic everywhere, with the possible exception of the real energy axis, and thus infinitely many times differentiable at any *complex* z), we observe that for $\partial\widetilde{\Sigma}(z)/\partial z$ to be unbounded at some *complex* z, it is necessary that $\widetilde{G}(z)$ should vanish at that z. Since $\widetilde{G}(z)$ does not vanish for any complex z (Subsec. 4.7), it follows that $\partial\widetilde{\Sigma}(z)/\partial z$ is bounded for *all* complex z. By differentiating both sides of Eq. (38) an arbitrary number of times, along the above line of reasoning we arrive at the conclusion that *nowhere on the physical RS, with the possible exception of the real axis, $\widetilde{\Sigma}(z)$ can be singular.*

Further, owing to the relations in Eqs. (39), (25) and (29), which equally hold for $G_0(\varepsilon)$ and $\widetilde{G}_0(z)$, we have (see DuBois 1959a, Appendix B; Luttinger 1961)

$$\Sigma(\mathbf{r},\mathbf{r}';\varepsilon) = \Sigma(\mathbf{r}',\mathbf{r};\varepsilon)\,; \quad \widetilde{\Sigma}(\mathbf{r},\mathbf{r}';z^*) = \widetilde{\Sigma}^*(\mathbf{r},\mathbf{r}';z)\,, \quad \mathrm{Im}(z) \neq 0\,. \tag{40}$$

Here the "physical" self-energy $\Sigma(\varepsilon)$ is defined through

$$\Sigma(\varepsilon) \equiv \lim_{\eta\downarrow 0} \widetilde{\Sigma}(\varepsilon \pm i\eta)\,, \quad \text{for } \varepsilon \gtrless \mu\,. \tag{41}$$

The analyticity of $\widetilde{\Sigma}(z)$ in the complex z-plane implies a pair of Kramers-Kronig-type relations (or Hilbert transforms — see Morse and Feshbach 1953, pp. 370–373 and 944) between the "real" and "imaginary" parts of $\widetilde{\Sigma}(z)$. In order to obtain these relations, it is required that we first establish the behaviour of $\widetilde{\Sigma}(z)$ for $|z| \to \infty$ (Farid 1999a). To this end let $\widetilde{f}(z) \sim f_0 + f_1/z + f_2/z^2 + \cdots$, for $|z| \to \infty$. Then provided $f_0 \neq 0$, it holds (Copson 1965, pp. 8 and 9): $1/\widetilde{f}(z) \sim 1/f_0 + \overline{f}_1/z + \overline{f}_2/z^2 + \cdots$, for $|z| \to \infty$, where $\overline{f}_1 = -f_1/f_0^2$, $\overline{f}_2 = (f_1^2 - f_0 f_2)/f_0^3$, etc. Through these results, making use of (*c.f.* Eq. (32)) $\widetilde{G}(z) \sim \hbar I/z + G_{\infty_2}/z^2 + \cdots$ and $\widetilde{G}_0(z) \sim \hbar I/z + G_{0;\infty_2}/z^2 + \cdots$, from the expression for $\widetilde{\Sigma}(z)$ in Eq. (39) we obtain the following general result

$$\widetilde{\Sigma}(z) \sim \Sigma_{\infty_0} + \frac{\Sigma_{\infty_1}}{z} + \frac{\Sigma_{\infty_2}}{z^2} + \cdots, \quad \text{as } |z| \to \infty. \tag{42}$$

Explicit calculation reveals that

$$\Sigma_{\infty_0} = \frac{1}{\hbar^2}\{-G_{0;\infty_2} + G_{\infty_2}\} \equiv \Sigma^{HF}, \tag{43}$$

the last relation being that given in Eq. (37).

The result in Eq. (43) can also be derived through analysing the Feynman diagrams for the SE operator. Briefly, due to the conservation of energy, all *skeleton* SE diagrams[26] (contributing to $\Sigma(\varepsilon)$) beyond the first order in the bare electron-electron interaction *inevitably* involve at least one GF whose energy argument contains ε. By "inevitably" we mean that it is not possible entirely to displace ε from the argument(s) of the GF(s) — through transformation of variables (or what is the same, reassigning energy variables in the diagrams) — to arguments of the electron-electron interaction function, which is independent of energy. This property holds true also for all those second and higher-order non-skeleton diagrams that do *not* contribute to the Fock diagram (a first-order diagram) in the process of partial summation of the non-skeleton diagrams, leading to the skeleton SE diagrams. Since we have $G(\varepsilon) \sim \hbar I/\varepsilon$ (for the case one employs non-skeleton SE diagrams, $G_0(\varepsilon) \sim \hbar I/\varepsilon$), for $|\varepsilon| \to \infty$, the integrands of these second- and higher-order SE contributions can be made as small as desired and thus only Σ^{HF} survives as the leading-order asymptotic term in the expansion of $\Sigma(\varepsilon)$ for large $|\varepsilon|$.

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[26] *Skeleton* diagrams (Luttinger and Ward 1960, Nozières 1964, p. 221) are those *proper* SE diagrams that do not contain any SE sub-diagrams that can be removed from them by "cutting" two GF lines. When in a perturbation expansion for the GF or the SE operator, skeleton diagrams are used, the directed lines in these that ordinarily would represent an unperturbed GF, G_0, must represent the full GF, G.

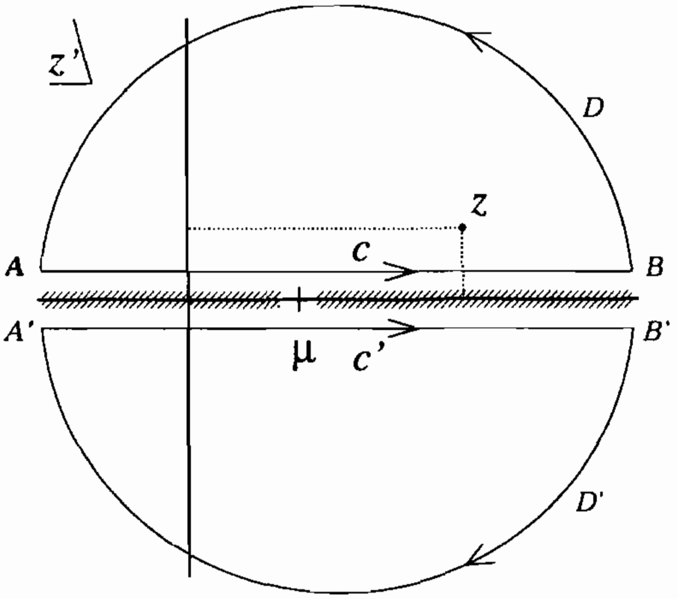

Fig. 5. The contours of integration employed for obtaining the Kramers-Kronig-type of relations for the *physical* self-energy operator $\Sigma(\varepsilon)$. The upper contonr is employed when $\mathrm{Im}(z) > 0$ (as in the Figure) and the lower contonr when $\mathrm{Im}(z) < 0$. It should be realised that when along $\overline{A'B'}$ and $\overline{AB}$ $\mathrm{Im}(z')$ is made to approach zero, *only* on sections $\overline{A'\mu}$ and $\overline{\mu B}$ one has $\widetilde{\Sigma}(z') \to \Sigma(\varepsilon')$.

From Eqs. (42) and (43) it follows that

$$\widetilde{\Sigma}_r(z) := \widetilde{\Sigma}(z) - \Sigma^{HF} \sim \frac{\Sigma_{\infty_1}}{z} + \frac{\Sigma_{\infty_2}}{z^2} + \cdots\,, \quad \text{for } |z| \to \infty\,. \tag{44}$$

Hence on integrating $\widetilde{\Sigma}_r(z')/(z'-z)$ along the contours C and C' in Fig. 5, the contributions of, respectively, the semi-circles $\overline{BDA}$ and $\overline{B'D'A'}$ to the total integral will become vanishingly small when the radii of the semi-circles are made infinitely large (and consequently $\overline{AB} \to (-\infty, \infty)$ and $\overline{A'B'} \to (-\infty, \infty)$). Now depending on whether $\mathrm{Im}(z) > 0$ or $\mathrm{Im}(z) < 0$, we carry out integration along C or C', respectively, and obtain (below $\eta' \downarrow 0$)

$$\widetilde{\Sigma}_r(z) = \frac{\pm 1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon' \frac{\widetilde{\Sigma}_r(\varepsilon' \pm i\eta')}{\varepsilon' - z}\,, \quad \mathrm{Im}(z) \gtrless 0\,. \tag{45}$$

In arriving at this expression we have made use of the Cauchy residue theorem (Titchmarsh 1939, p. 102), relying on the fact that $\widetilde{\Sigma}_r(z')$, similar to $\widetilde{\Sigma}(z')$, is, with the possible exception of the real energy axis, analytic everywhere on the physical RS. Through substituting $z = \varepsilon \pm i\eta$, with $\eta \downarrow 0$, in Eq. (45), making use of $1/(x - x_0 \pm i\eta) = \mathcal{P}(1/[x - x_0]) \mp i\pi\delta(x - x_0)$ we obtain

$$\widetilde{\Sigma}_r(\varepsilon \pm i\eta) = \pm\frac{1}{\pi i}\mathcal{P}\int_{-\infty}^{\infty} d\varepsilon' \frac{\widetilde{\Sigma}_r(\varepsilon' \pm i\eta)}{\varepsilon' - \varepsilon}\,. \tag{46}$$

Let

$$\widetilde{\Sigma}'_r(z) := \frac{1}{2}\{\widetilde{\Sigma}_r(z) + \widetilde{\Sigma}_r^{\dagger}(z)\}\,, \quad \text{and} \quad \widetilde{\Sigma}''_r(z) := \frac{1}{2i}\{\widetilde{\Sigma}_r(z) - \widetilde{\Sigma}_r^{\dagger}(z)\} \tag{47}$$

be the "real" and "imaginary" parts of $\widetilde{\Sigma}_r(z)$.[27] The result in Eq. (46) can be written as the following pair of the Kramers-Kronig-type expressions

$$\begin{aligned} \widetilde{\Sigma}'_r(\varepsilon \pm i\eta) &= \pm\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\varepsilon' \frac{\widetilde{\Sigma}''_r(\varepsilon' \pm i\eta)}{\varepsilon' - \varepsilon}\,, \\ \widetilde{\Sigma}''_r(\varepsilon \pm i\eta) &= \mp\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\varepsilon' \frac{\widetilde{\Sigma}'_r(\varepsilon' \pm i\eta)}{\varepsilon' - \varepsilon}\,. \end{aligned} \tag{48}$$

This pair is easily verified correctly to conform with the exact relations

$$\widetilde{\Sigma}'_r(z^*) = \widetilde{\Sigma}'_r(z)\,, \quad \widetilde{\Sigma}''_r(z^*) = -\widetilde{\Sigma}''_r(z)\,, \tag{49}$$

which are direct consequences of $\widetilde{\Sigma}_r^{\dagger}(z) \equiv \widetilde{\Sigma}_r(z^*)$ — *c.f.* Eq. (40). We remark that the expressions in Eq. (48) are not in terms of solely the *physical* SE. For obtaining a pair of expressions entirely in terms of the latter, we make use of Eq. (49). After some algebra, from Eq. (48) the desired Kramers-Kronig-type of relations for the *physical* SE operator (see Eq. (41)) are shown to be

$$\begin{aligned} \Sigma'_r(\varepsilon) &= -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\varepsilon' \frac{\mathrm{sgn}(\mu - \varepsilon')\Sigma''_r(\varepsilon')}{\varepsilon' - \varepsilon}\,, \\ \Sigma''_r(\varepsilon) &= \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\varepsilon' \frac{\mathrm{sgn}(\mu - \varepsilon)\Sigma'_r(\varepsilon')}{\varepsilon' - \varepsilon}\,. \end{aligned} \tag{50}$$

Finally, according to a theorem due to Luttinger and Ward (1960), the following relations (one obtained from the other through integration by parts

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[27] We have to emphasise that $\widetilde{\Sigma}_r(z)$ is an *operator* so that $\widetilde{\Sigma}'_r(z)$ and $\widetilde{\Sigma}''_r(z)$ may *not* be real-valued in specific representations — in addition, upon a gauge transformation, a real-valued representation of, say, $\widetilde{\Sigma}'_r(z)$, can easily be made complex-valued. This comment applies to all other operators, like $\widetilde{\chi}'(z)$ and $\widetilde{\chi}''(z)$, that we encounter in the present work — note, however, that contrary to G, χ is gauge invariant.

— the asymptotic behaviour of the functions involved lead to vanishing end-point contributions) are satisfied

$$\int_{\mu-i\infty}^{\mu+i\infty} dz\widetilde{G}(z)\frac{\partial\widetilde{\Sigma}(z)}{\partial z} \equiv -\int_{\mu-i\infty}^{\mu+i\infty} dz\widetilde{\Sigma}(z)\frac{\partial\widetilde{G}(z)}{\partial z} = 0\,. \tag{51}$$

Although for the exact $\widetilde{G}(z)$ and $\widetilde{\Sigma}(z)$ these expressions amount to identities, in approximate frameworks these can best be violated (see Subsec. 9.2). Therefore Eq. (51) lends itself for use as a "self-consistency" condition in approximate calculations.[28] The expressions in Eq. (51) are closely related to the Friedel sum-rule for *interacting* electrons (Langer and Ambegaokar 1961).

5.2. *A "local-density" approximation for* $\Sigma(\varepsilon)$

Sham and Kohn (1966) have shown that at least for systems with almost uniform electronic density (such as ideal metals), $\Sigma(\mathbf{r},\mathbf{r}';\varepsilon)$ has an interesting short-range property. By writing $\Sigma(\mathbf{r},\mathbf{r}';\varepsilon) = \hbar^{-1}v_H(\mathbf{r};[n])\delta(\mathbf{r}-\mathbf{r}') + M(\mathbf{r},\mathbf{r}';\varepsilon - v_H(\mathbf{r}_0;[n]))$, where $\mathbf{r}_0 := (\mathbf{r}+\mathbf{r}')/2$, these authors have shown that owing to one of the Ward identities (corresponding to the long wavelength behaviour of the static density-density correlation function), $\delta M\big(\mathbf{r},\mathbf{r}';\varepsilon - v_H(\mathbf{r}_0;[n])\big)/\delta n(\mathbf{r}'')$, taken at the uniform density n, is a relatively short-ranged function of $\mathbf{r}_0-\mathbf{r}''$, implying that the difference between $M(\mathbf{r},\mathbf{r}';\varepsilon - v_H(\mathbf{r}_0;[n]))$, pertaining to the *inhomogeneous* system (with almost constant density) and $M_h(\mathbf{r}-\mathbf{r}';\varepsilon - v_H(\mathbf{r}_0[n]);n)$, pertaining to the *uniform*-electron system,[29] is mainly determined by the deviation from the average value of the charge density in the close vicinity of $\mathbf{r}_0$. This finding has been the basis for construction of the following "local-density approximation" for the SE operator (Sham and Kohn 1966)

$$\Sigma^{LDA}(\mathbf{r},\mathbf{r}';\varepsilon) := \frac{1}{\hbar}v_H(\mathbf{r};[n])\delta(\mathbf{r}-\mathbf{r}') + M_h(\mathbf{r}-\mathbf{r}';\varepsilon - v_H(\mathbf{r}_0;[n]);n(\mathbf{r}_0))\,,$$

$$\mathbf{r}_0 := \frac{1}{2}(\mathbf{r}+\mathbf{r}')\,. \tag{52}$$

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[28] In this connection we should like to emphasise that the Dyson *equation* (see Eq. (38)), in reality is also an *identity*, expressing a relationship amongst the *exact* G, G_0 and the corresponding *exact* Σ. It becomes an *equation*, however, when either G or Σ is approximated (in the former case an *equation* for Σ and in the latter an *equation* for G).

[29] Here the last argument n denotes the *constant* density of the system to which M_h corresponds.

For some discussions concerning this approximation see (Hedin and Lundqvist 1969). This approximation has been applied by Wang and Pickett (1983) and Pickett and Wang (1984) and more recently by Engel and Pickett (1996).

6. Quasi-Particles; Particle-Like Excitations

In this Section we present a framework within which the information contained in the single-particle Green function concerning the single-particle excitation energies of interacting systems is abstracted. We show that a one-electron-like Schrödinger equation, the quasi-particle equation, should yield the energies and the associated "wavefunctions" of the quasi-particles. Close inspection of the analytic properties of the energy-dependent potential (i.e. the SE operator) in this equation reveals, however, that without an analytic continuation of this potential into a non-physical RS, this equation *in general* does not have any solution for systems in the thermodynamic limit (Farid 1999a).

Consider the Dyson equation in Eq. (38) which can be solved for $\widetilde{G}(z)$ as follows

$$\widetilde{G}(z) = \left(I - \widetilde{G}_0(z)\widetilde{\Sigma}(z)\right)^{-1} \widetilde{G}_0(z) = \widetilde{G}_0(z) + \widetilde{G}_0(z)\widetilde{\Sigma}(z)\widetilde{G}_0(z) + \cdots , \quad (53)$$

where the last series represents merely a *formal* solution, as it may not be convergent. This series can be viewed as a perturbation series for $\widetilde{G}(z)$ in terms of $\widetilde{G}_0(z)$, with $\widetilde{\Sigma}(z)$ acting as the perturbation. Analogous to the case in which the convergence towards $1/(1-z) =: \widetilde{f}(z)$ of the simple geometric series $1 + z + z^2 + \cdots$ is hampered by the singularity (here, a simple pole) of $\widetilde{f}(z)$ at $z = 1$, convergence of the series on the RHS of Eq. (53) is restricted by the singular points of the exact GF (see Subsecs. 4.1 and 4.5). In Subsec. 4.1 we have seen that these singularities ("poles") are the one-particle excitation energies of the interacting N-particle system (i.e. the energies of the interacting ground and excited $N \pm 1$-particle states relative to the energy of the interacting GS of the N-particle state). Hence the series on the RHS of Eq. (53) diverges at these excitation energies. This happens when

$$\det(I - \widetilde{G}_0(z)\widetilde{\Sigma}(z)) = 0 , \quad (54)$$

which should be compared with the condition $1/\widetilde{f}(z) = 0$ (*c.f.* the first expression on the RHS of Eq. (53)). The GF $\widetilde{G}_0(z)$ satisfies

$$(zI - H_0)\widetilde{G}_0(z) = \hbar I . \quad (55)$$

Suppose that z does not coincide with a "pole" of $\widetilde{G}_0(z)$, that is z is not equal to a one-particle excitation energy of the non-interacting system described by H_0, or, what is the same, $\det(zI - H_0) \neq 0$. In this case we can write Eq. (54) in the alternative and equivalent form $\det(\widetilde{G}_0^{-1}(z) - \widetilde{\Sigma}(z)) = 0$, or

$$\det(zI - [H_0 + \hbar\widetilde{\Sigma}(z)]) = 0\,. \tag{56}$$

The possible solutions $z = z_s$ of this equation are eigenvalues of the (in general) non-Hermitian "quasi-particle" Hamiltonian

$$\widetilde{\mathcal{H}}_{qp}(z) := H_0 + \hbar\widetilde{\Sigma}(z). \tag{57}$$

The non-Hermiticity of $\widetilde{\mathcal{H}}_{qp}(z)$ implies that its set of right eigenfunctions $\{\widetilde{\psi}_s(z)\}$ is not orthogonal. It can however be shown (Morse and Feshbach 1953, pp. 884–886) that when the sets of *left* and *right* eigenfunctions of $\widetilde{\mathcal{H}}_{qp}(z)$, $\{\widetilde{\phi}_s(z)\}$ and $\{\widetilde{\psi}_s(z)\}$, respectively, have been arranged in such a way that $\phi_s(z)$ and $\widetilde{\psi}_s(z)$ correspond to the *same* eigenvalue $\widetilde{E}_s(z)$, i.e.[30]

$$\widetilde{\mathcal{H}}_{qp}(z)\widetilde{\psi}_s(z) = \widetilde{E}_s(z)\widetilde{\psi}_s(z)\,, \tag{58}$$

$$\widetilde{\phi}_s^\dagger(z)\widetilde{\mathcal{H}}_{qp}(z) = \widetilde{E}_s(z)\widetilde{\phi}_s^\dagger(z) \iff \widetilde{\mathcal{H}}_{qp}^\dagger(z)\widetilde{\phi}_s(z) = \widetilde{E}_s^*(z)\widetilde{\phi}_s(z)\,, \tag{59}$$

then for $\widetilde{E}_s(z) \neq \widetilde{E}_{s'}(z)$, $\langle\widetilde{\phi}_s(z), \widetilde{\psi}_{s'}(z)\rangle = \delta_{s,s'}$ (here we have assumed normalisation to *unity*). In the case of degeneracy, i.e. $\widetilde{E}_s(z) = \widetilde{E}_{s'}(z)$ for $s \neq s'$, the degenerate left and right eigenfunctions can be made orthogonal through a Gram-Schmidt orthogonalisation procedure, however, it is possible that the resulting left and right eigenvectors may not span the original space (Goldenfeld 1992, p. 255) — see further on as well as Appendix A. From Eq. (56) it follows that for the eigenvalues (eigenfunctions) of Eq. (58) to coincide with the QP "energies" ("wavefunctions") it must hold

$$\widetilde{E}_s(z) = z\,; \tag{60}$$

with this, Eq. (56) turns into $\det(\widetilde{E}_s(z)I - \widetilde{\mathcal{H}}_{qp}(z)) = 0$. We thus refer to Eq. (60) as the equation for the QP energies.

From the above considerations it follows that $\widetilde{\mathcal{H}}_{qp}(z)$ can be expressed in the following bi-ortho*normal* spectral representation

$$\widetilde{\mathcal{H}}_{qp}(\mathbf{r}, \mathbf{r}'; z) = \sum_s \widetilde{E}_s(z)\widetilde{\psi}_s(\mathbf{r}; z)\widetilde{\phi}_s^*(\mathbf{r}'; z)\,. \tag{61}$$

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[30] It can be shown (Morse and Feshbach 1953, p. 885) that sets of *left* and *right* eigenvalues are, up to ordering, identical.

Because of the properties presented in Eq. (40), from $\langle \mathbf{r}|\widetilde{\Sigma}^{\dagger}(z)|\mathbf{r}'\rangle \equiv \langle \mathbf{r}'|\widetilde{\Sigma}(z)|\mathbf{r}\rangle^{*}$ it follows that

$$\widetilde{\phi}_s(\mathbf{r};z) = \widetilde{\psi}_s(\mathbf{r};z^{*})\,, \quad \widetilde{\psi}_s(\mathbf{r};z) = \widetilde{\phi}_s(\mathbf{r};z^{*})\,, \quad \widetilde{E}_s(z^{*}) = \widetilde{E}_s^{*}(z)\,. \tag{62}$$

We have, moreover (*c.f.* Subsec. 4.4), that for every s there exists an $\bar{s}$ such that $\widetilde{E}_{\bar{s}}(z) = \widetilde{E}_s(z)$, Kramers' degeneracy (Subsec. 4.4), and that $\widetilde{\psi}_{\bar{s}}(\mathbf{r};z) = e^{i\theta_s}\widetilde{\phi}_s^{*}(\mathbf{r};z)$ and $\widetilde{\phi}_{\bar{s}}(\mathbf{r};z) = e^{i\theta_s}\widetilde{\psi}_s^{*}(\mathbf{r};z)$. Thus the bi-orthonormal spectral representation in Eq. (61) indeed preserves the symmetry property $\widetilde{\mathcal{H}}_{qp}(\mathbf{r},\mathbf{r}';z) = \widetilde{\mathcal{H}}_{qp}(\mathbf{r}',\mathbf{r};z)$. From the above results we also infer that $\widetilde{\psi}_{\bar{s}}(\mathbf{r};z) = e^{i\theta_s}\widetilde{\psi}_s(\mathbf{r};z^{*})$ and $\widetilde{\phi}_{\bar{s}}(\mathbf{r};z) = e^{i\theta_s}\widetilde{\phi}_s(\mathbf{r};z^{*})$.

In view of our earlier remark concerning the fact that in the event of degeneracy the left and right eigenvectors are *not* necessarily orthogonal, and in view of the above-mentioned Kramers' degeneracy of the QP states labelled by s and $\bar{s}$, $s \neq \bar{s}$, the following remark is in place. In systems with some spatial symmetry (such as translation symmetry, whether continuous or discrete), by choosing the left and right eigenvectors to be simultaneously basis functions for the unitary irreducible representations of the pertinent symmetry group, the degenerate left and right eigenvectors will be automatically orthogonal when they belong to different unitary irreducible representations (Cornwell 1984, pp. 81–83). This is the case, for instance, for the non-interacting uniform-electron system (see the closing paragraph in Subsec. 4.4) where the Kramers degenerate states corresponding to $-\mathbf{k}$ and $\mathbf{k}$ (recall that $\varepsilon_{-\mathbf{k}}^{0} = \varepsilon_{\mathbf{k}}^{0}$) are automatically orthogonal, owing to the fact that for $\mathbf{k} \neq \mathbf{0}$, $-\mathbf{k}$ and $\mathbf{k}$ mark two distinct unitary irreducible representations of the continuous translation group.

Using the operator relation $(AB)^{-1} = B^{-1}A^{-1}$ and the first term on the RHS of Eq. (53), it follows that $\widetilde{G}(z) = \hbar(zI - \widetilde{\mathcal{H}}_{qp}(z))^{-1}$, so that by completeness relation $\sum_s \widetilde{\psi}_s(z)\widetilde{\phi}_s^{\dagger}(z) = I$ [in the coordinate representation $\sum_s \widetilde{\psi}_s(\mathbf{r};z)\widetilde{\phi}_s^{*}(\mathbf{r}';z) = \delta(\mathbf{r}-\mathbf{r}')$] and Eq. (61) we obtain the following bi-ortho*normal* representation for $\widetilde{G}(z)$ — (Layzer 1963):

$$\widetilde{G}(\mathbf{r},\mathbf{r}';z) = \hbar \sum_s \frac{\widetilde{\psi}_s(\mathbf{r};z)\widetilde{\phi}_s^{*}(\mathbf{r}';z)}{z - \widetilde{E}_s(z)}\,. \tag{63}$$

This representation makes explicit that Eq. (60), i.e. the equation for the QP energies, coincides with the equation for the "zeros" of the denominator in Eq. (63), or that for "poles" of $\widetilde{G}(z)$. Note that because the functions $\widetilde{\psi}_s(z)$

and $\widetilde{\phi}_s(z)$ are *normalised* for *all* values of z, i.e. $\langle\widetilde{\phi}_s(z), \widetilde{\psi}_{s'}(z)\rangle = \delta_{s,s'}$, the "poles" of $\widetilde{G}(z)$ cannot be due to the functions in the numerator in Eq. (63).

The regularity of $\widetilde{\Sigma}(z)$ on the physical RS (see Subsec. 5.1) has some interesting consequences. For instance, from Eq. (57) we observe that $\widetilde{\mathcal{H}}_{qp}(z)$ is analytic in exactly the same region of the z-plane where $\widetilde{\Sigma}(z)$ is analytic. This, through Eq. (58), or Eq. (59), implies that $\widetilde{E}_s(z)$ is analytic everywhere on the physical RS, with the possible exception of the real axis (recall that the left and right eigenstates of $\widetilde{\mathcal{H}}_{qp}(z)$ are bounded through normalisation). We point out that if $\widetilde{E}_s(z)$ were unbounded at some *complex* z, say at $z = z_0$, then form Eq. (63) it would follow that $\widetilde{G}(z)$ would be vanishing at $z = z_0$, which contradicts the finding in Subsec. 4.7.

For our further discussions we define

$$\widetilde{E}'_s(z) := \frac{1}{2}\{\widetilde{E}_s(z) + \widetilde{E}^*_s(z)\}, \quad \widetilde{E}''_s(z) := \frac{1}{2i}\{\widetilde{E}_s(z) - \widetilde{E}^*_s(z)\}. \tag{64}$$

The 'physical' $E_s(\varepsilon)$ is obtained from

$$E_s(\varepsilon) = \lim_{\eta\downarrow 0} \widetilde{E}_s(\varepsilon \pm i\eta), \quad \varepsilon \gtrless \mu. \tag{65}$$

Through comparing the representation in Eq. (63) with the Lehmann representation in Eq. (11), we deduce the following conditions:[31]

$$E''_s(\varepsilon) \lesseqgtr 0, \quad \text{for} \quad \varepsilon \gtrless \mu. \tag{66}$$

Violation of these inequalities signifies breakdown of the causality, or instability of the GS due to its collapse into a lower-energy state.

From the second expression in Eq. (64) and the last expression in Eq. (62) it is evident that for $\mathrm{Im}(z) \to 0$, $\widetilde{E}''_s(z)$ measures the amount of discontinuity in $\widetilde{E}_s(z)$ across its possible branch cuts along the real energy axis. It is obvious that unless $E''_s(\varepsilon) = 0$, Eq. (60) for the QP energies, i.e. $E_s(\varepsilon) = \varepsilon$, *cannot* be satisfied. For systems in the thermodynamic limit, $E''_s(\varepsilon)$ is non-vanishing, except for isolated regions of the real axis. Therefore, for these systems the QP equation in general does not have real-valued solutions; such solutions can only occur on the mentioned isolated intervals of the real energy axis. As for the complex-valued solutions, these are excluded by the fact that $\widetilde{G}(z)$ is

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[31] Despite the similarities between the Lehmann representation in Eq. (11) and the bi-orthonormal representation in Eq. (63), the two are *not* identical; they are, however, both exact.

analytic for *all* z, with $\mathrm{Im}(z) \neq 0$ (see Sec. 5.1). Alternatively, owing to the reflection property $\widetilde{E}_s(z^*) = \widetilde{E}_s^*(z)$ given in Eq. (62), a solution at $z = z_0$, with $\mathrm{Im}(z_0) \neq 0$, would imply one at $z = z_0^*$, which is in violation of causality. The possible complex-valued solutions of Eq. (60) must therefore be sought on the non-physical RSs (Subsec. 2.2). This requires analytic continuation of $\widetilde{E}_s(z)$ into these non-physical RSs. This can be achieved through a Taylor expansion of $\widetilde{E}_s(z)$ around $z = z_0$ with $\mathrm{Re}(z_0) > \mu$ and $\mathrm{Im}(z_0) > 0$ *or* $\mathrm{Re}(z_0) < \mu$ and $\mathrm{Im}(z_0) < 0$. Suppose $\mathrm{Re}(z_0) > \mu$ and $\mathrm{Im}(z_0) > 0$. Provided $\mathrm{Re}(z_0)$ does not coincide with the location of a singularity of $\widetilde{E}_s(z)$ on the real energy axis, this expansion yields $\tilde{\tilde{E}}_s(z)$, the analytic continuation of $\widetilde{E}_s(z)$ from the first quadrant of the physical RS into the fourth quadrant of a non-physical RS directly beneath the physical RS. This continuation is valid within a circular disk, centred around $z = z_0$, whose radius is equal to the distance between z_0 and the singularity of $\widetilde{E}_s(z)$ on the real axis which is closest to z_0. If $\tilde{\tilde{E}}_s(z) = z$ is satisfied within this disk, then evidently the imaginary part of the solution (or solutions), say z_s (or z_{s_j}'s), is (are) finite and negative. In view of the fact that $\widetilde{E}_s(z_s) \neq z_s$ (or $\widetilde{E}_s(z_{s_j}) \neq z_{s_j}$ — note the number of tildes), the existence of a z_s (or z_{s_j}'s) satisfying $\tilde{\tilde{E}}_s(z) = z$, is *not* in contradiction with the stability of the system as well as with causality.

Complex QP energies z_s, corresponding to damped one-particle-like excitations, signify the irreversibility of the process of evaluating the thermodynamic limit. For systems classified as Landau Fermi liquids (see Subsec. 6.3) one finds real-valued solutions for the QP equation, Eq. (60). However, these solutions do *not* correspond to *poles* of $\widetilde{G}(z)$ but to non-isolated singularities (Subsec. 2.1). As we shall discuss in Subsecs. 6.2 and 6.3, these singularities can be considered as poles only in an asymptotic sense.

Finally, since the non-Hermiticity of the physical SE operator — in its seeming similarity with the optical-model potential (Schiff 1968, pp. 129 and 130, Landau and Lifshitz 1977, pp. 613 and 614) — may suggest lack of energy conservation in the system, we mention that the finite life-times of the QPs (or what is the same, the finite imaginary parts of the QP energies), are *not* due to lossy processes (such as *inelastic* scattering processes with impurity potentials). Rather, it signifies the fact that elementary excitations of macroscopic systems in general do not behave like stable particles over long time intervals: due to the electron-electron interaction and abundance of energy levels in such systems (see Sec. 1), any energetically sharply defined initial excitation in the system will, in general, lose its energy to other allowed excitations in the system, in such a way that the total energy of the system retains its constant value in the course of time. It should be noted that here the *thermodynamic limit* plays a crucial role, since prior to taking this limit, one would be able in principle to excite a single eigenstate of the system, which in the ideal case would remain stationary for an indefinite duration of time.[32]

6.1. *The quasi-particle approximation*

In Sec. 6 we observed that the possible solutions of $\widetilde{E}_s(z) = z$ are the energies of un-damped one-particle excitations of the interacting N-electron system, i.e. the energies of undamped QPs. For systems in the thermodynamic limit such solutions, if at all existent, describe only a negligible part of the structure that one observes in, for instance, the photo-emission or inverse photo-emission spectra. Here we will elaborate on issues that link theory with experiment.

Consider the spectral function as defined in Eq. (30) and calculated in terms of the bi-orthonormal representation for the GF in Eq. (63) (see Eq. (65)),

$$A_p(\mathbf{r},\mathbf{r}';\varepsilon) = \frac{-\hbar}{\pi} \sum_s \widetilde{\psi}_s(\mathbf{r};\varepsilon + \mathrm{sgn}[\varepsilon-\mu]i\eta)\widetilde{\phi}_s^*(\mathbf{r}';\varepsilon + \mathrm{sgn}[\varepsilon-\mu]i\eta)$$

$$\times \operatorname{Im}\left\{\frac{1}{\varepsilon - E_s(\varepsilon)}\right\}, \quad (\eta \downarrow 0)\,. \tag{67}$$

In arriving at Eq. (67) we have made use of the expressions in and following Eq. (62). It is the behaviour of this function along the (real) energy axis that is to be compared with experimentally-measured one-particle spectra. Often, however, the experimental data are not spatially fully resolved, so that for comparison with these data, some part of the spatial information contained in $A_p(\mathbf{r},\mathbf{r}';\varepsilon)$ has to be integrated out. This is best done by first Fourier transforming the spectral function into the wave-vector space (see Appendix A), which is suitable from the experimental point of view, since far (on atomic scale) outside the sample, momentum is a good quantum number (one may think of the angle-resolved photo-emission experiments, whereby the dispersions of the QP-energy bands as functions of the wave-vector of the incident particle can be measured); see Cohen and Chelikowsky (1988). Let us for the moment neglect the entire spatial or wave-vector resolution through equating $\mathbf{r}'$ in $A_p(\mathbf{r},\mathbf{r}';\varepsilon)$ with $\mathbf{r}$ and integrating $\mathbf{r}$ over the normalisation space of

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[32] In practice, however, the coupling between the field of the electrons and the free electromagnetic field in vacuum, or, in solids, the field of phonons (both of which we have neglected in our considerations), renders even these excitations non-stationary.

$\{\widetilde{\psi}_s(\mathbf{r};z)\}$ and $\{\widetilde{\phi}_s(\mathbf{r};z)\}$. Because of the bi-ortho-normality of $\{\widetilde{\psi}_s(z)\}$ and $\{\widetilde{\phi}_s(z)\}$ (see text following Eq. (59)) one obtains

$$\mathcal{D}(\varepsilon) := \frac{-\hbar}{\pi}\sum_s \mathrm{Im}\left\{\frac{1}{\varepsilon - E_s(\varepsilon)}\right\}, \tag{68}$$

which for "non-interacting" systems (i.e. those for which the SE operator is energy independent and Hermitian) reduces to the well-known electronic *density of states* (DOS) (or *density of levels*), concerning both "occupied" ($\varepsilon < \mu$) and "unoccupied" ($\varepsilon > \mu$) states. This is easily seen by employing $\mathrm{Im}\{1/(x - x_0 \pm i\eta)\} = \mp\pi\delta(x - x_0)$, for $\eta \downarrow 0$.

Equation (68) suggests that the peak structure observed in $\mathcal{D}(\varepsilon)$ for certain values of energy ε, corresponds to those energies which satisfy the following set of requirements (see Eqs. (64) and (65)):

$$\begin{aligned} E_s'(\varepsilon) &= \varepsilon\,, \\ \partial E_s''(\varepsilon)/\partial\varepsilon &= 0\,, \\ \partial^2 E_s''(\varepsilon)/\partial\varepsilon^2 &\gtrless 0\,, \quad \text{for } \varepsilon \gtrless \mu\,. \end{aligned} \tag{69}$$

These ε's may be termed the "experimental quasi-particle energies", as at these ε's the *amplitude* of the DOS is maximal. We point out that when a solution of the first of the above three requirements satisfies $E_s''(\varepsilon) = 0$, the remaining two conditions must be relaxed since this solution coincides with the energy of an un-damped QP in the system. Further, the second and third of the above expressions are merely *formal* statements indicating that at the "experimental" quasi-particle energies, $|E_s''(\varepsilon)|$ is *minimal*. This observation is important from the point of view of the fact that $E_s''(\varepsilon)$ may *not* be differentiable. This is the case for instance at the "band edges" and at the locations of the van Hove singularities, which are branch points (Subsec. 2.1) of $\widetilde{E}_s(z)$ along the real energy axis (see Subsecs. 6.2 and 6.5).

In cases where $\widetilde{E}_s(z)$ is free from branch points in the neighbourhood of an "experimental" QP energy, say ε_s^{ex}, through Taylor expanding $\widetilde{E}_s(z)$ around $z = \varepsilon_s^{ex}$, one obtains the analytic continuation of $\widetilde{E}_s(z)$ into a limited region of a non-physical RS (see Subsecs. 2.3 and 2.4). Denoting this analytic continuation by $\widetilde{\widetilde{E}}_s(z)$, one can subsequently seek to solve $\widetilde{\widetilde{E}}_s(z) = z$. Because $\widetilde{\widetilde{E}}_s(z)$ has been obtained through an analytic continuation around an "experimental" QP energy, it is likely that the latter equation indeed has a solution close to the real energy axis. Let this solution be denoted by z_s. We indicate the union of the "energy" function that on the non-physical RS coincides with $\widetilde{\widetilde{E}}_s(z)$ and on the physical RS with $\widetilde{E}_s(z)$ by $\mathcal{E}_s(z)$ (this is the equivalent of $\mathcal{F}(z)$ in Subsec. 2.2). Now let us Taylor expand $\mathcal{E}_s(z)$ around $z = z_s$. Since $\mathcal{E}_s(z_s) = z_s$, within a certain region around $z = z_s$ we have: $\mathcal{E}_s(z) = z_s + \partial\mathcal{E}_s(z)/\partial z|_{z=z_s}(z - z_s) + \mathcal{O}((z - z_s)^2)$, so that for z on the physical RS in the neighbourhood of $z = \varepsilon_s^{ex}$ we can write

$$\frac{1}{z - \widetilde{E}_s(z)} \approx \frac{g_s}{z - z_s}, \quad \text{for sufficiently small } |z - z_s|, \tag{70}$$

where

$$g_s := \left(1 - \left.\frac{\partial\mathcal{E}_s(z)}{\partial z}\right|_{z=z_s}\right)^{-1}. \tag{71}$$

Note the occurrence of $\mathcal{E}_s(z)$, and *not* of $\widetilde{E}_s(z)$, in the definition for g_s; as should be clear, at $z = z_s$ it is $\mathcal{E}_s(z)$, or equivalently $\widetilde{\widetilde{E}}_s(z)$, that satisfies $\mathcal{E}_s(z) = z$ and *not* $\widetilde{E}_s(z)$. Only when z_s is real-valued, that is when $z_s = \varepsilon_s^{ex}$, or in other words, when $E_s(\varepsilon_s) = \varepsilon_s$, can one replace $\mathcal{E}_s(z)$ by $\widetilde{E}_s(z)$. Suppose now that g_s were real-valued. By multiplying the RHS of Eq. (70) by $1 \equiv (z-z_s)^*/(z-z_s)^*$, it follows that for $z = \varepsilon \pm i\eta$, the imaginary part of $1/(z - E_s(\varepsilon))$ would be approximately a Lorentzian (*c.f.* Eq. (68)), with $\mathrm{Im}(z_s)$ being its width at half maximum. Since $\hbar/[2\mathrm{Im}(z_s)]$ can be viewed as the life-time[33] of the QP with energy $\mathrm{Re}(z_s)$, we observe that the width of a peak in $\mathcal{D}(\varepsilon)$, or indeed $A_p(\varepsilon)$, can be associated to the life-time of the QP whose (real) energy coincides with the location of the peak along the ε-axis. For *real* values of g_s holds: $0 \le g_s \le 1$ if $\partial\widetilde{E}_s(z)/\partial z|_{z=\varepsilon_s^{ex}} \le 0$, and $g_s > 1$ if $0 < \partial\widetilde{E}_s(z)/\partial z|_{\varepsilon=\varepsilon_s^{ex}} < 1$.[34]

Three remarks are in place. First, $\mathcal{E}_s(z) = z$ may have more than one solution inside the domain of definition of $\mathcal{E}_s(z)$ (these solutions may be denoted by z_{s_j}, $j = 1, 2, \dots, n_s$). In the case $n_s > 1$, the expression in Eq. (70) must accordingly be modified. When of the possible n_s (> 1) solutions, m_s ($\le n_s$)

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[33] The factor 2 in $\tau_s := \hbar/[2\mathrm{Im}(z_s)]$ originates from the fact that it is $|\widetilde{\psi}_s(z_s)|^2$ (note the power 2) that describes the probability density of the QP associated with $\widetilde{\psi}_s(z_s)$.

[34] For g_s pertaining to a QP on the Fermi surface, i.e. Z_{k_F}, holds $0 \le Z_{k_F} \le 1$. The property $|Z_{k_F}| \le 1$ follows from the fact that by definition $0 \le \mathsf{n}(k) \le 1$ (see Eq. (83)) and that according to a Migdal's theorem, to be discussed in Subsec. 6.6, $Z_{k_F} = \mathsf{n}(k_F^-) - \mathsf{n}(k_F^+)$ (see Eq. (85)); $Z_{k_F} \ge 0$ reflects the property $\Sigma''(k;\varepsilon) \gtrless 0$ for $\varepsilon \gtrless \mu$. We emphasise that $Z_{k_F} = 0$ does *not* imply absence of the Fermi surface; see text following Eq. (81) and Footnote 40.

coincide, the Taylor expansion of $\mathcal{E}_s(z)$ around this multiple solution (from which expansion, in the case of $n_s = 1$, Eq. (70) has been obtained) must be continued up to and including the m_sth order. Second, the pole in the expression on the RHS of Eq. (70) can *never* lie on the physical RS, since, unless z_s be real-valued, z_s can *never* satisfy $\widetilde{E}_s(z) = z$. Third, when z_s is complex-valued, the approximation in Eq. (70) breaks down for those points on the physical RS that lie outside the radius of convergence of the Taylor expansion of $\mathcal{E}_s(z)$ around $z = z_s$. The severity of the consequences of this failure, on the calculated low-energy properties,[35] depends on how large the ratio $\mathrm{Im}(z_s)/\mathrm{Re}(z_s)$ is. The smaller this ratio, the less severe are the consequences.

When the entire peak structure in $A_p(\varepsilon)$, or $\mathcal{D}(\varepsilon)$, or indeed $G(\varepsilon)$, is subjected to the approximation in Eq. (70), then the resulting expression is referred to as the "quasi-particle approximation" for $A_p(\varepsilon)$, etc. Although possibly reasonably accurate for certain regions of energy, this approximation is in general poor. In particular, strict adherence to it gives rise to violation of very fundamental energy ("frequency") sum-rules (see, e.g., Eq. (34) above).

6.2. *Quasi-particle energies: Poles and non-isolated singularities*

Above we have established that equation $\widetilde{E}_s(z) = z$ has either no solution, or if it has one (or some), this (these) must be real-valued. Now it may happen that while $\widetilde{E}_s(z) = z$ has a *real-valued* solution, this coincides with a singular point[36] of $\widetilde{E}_s(z)$. In such an event, one must realise that the QP approximation described in Subsec 6.1 may break down, in which case the approximation presented in Eq. (70) and, in particular, such quantity as g_s in Eq. (71) becomes meaningless. Let us illustrate this situation by means of a simple example. Consider $f(x) := (x-1)^{1/2} + 1$ whose analytic continuation into the complex z-plane is $\widetilde{f}(z) = (z-1)^{1/2}+1$. This functions has two branch points, one at $z = 1$ and the other at the point of infinity (Subsec. 2.1), i.e. at $1/z = 0$. We cut the complex plane along $(-\infty, 1]$, and of the two branches choose the one for which holds $\widetilde{f}(x) = f(x)$ for $x > 1$; this is what defines

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[35] For instance, application of the approximation in Eq. (70) to the low-energy peak structures in $\mathcal{D}(\varepsilon)$ pertaining to a semiconductor or insulator leads to a non-vanishing density of levels inside the QP gap.

[36] Recall that (Subsec. 2.1) when, say, $g(z)$ is *analytic* at $z = z_0$, z_0 is interior to an open region in which $g(z)$ is regular. The same is valid when z_0 is an *isolated* singularity of $g(z)$: there exists an open neighbourhood of z_0 where z_0 is the *only* singularity of $g(z)$. Branch points of $g(z)$, by definition, cannot be interior to any open region in which $g(z)$ would be analytic.

$\widetilde{f}(z)$; the other branch, according to the notational convection adopted in this work, should be denoted by $\widetilde{\widetilde{f}}(z)$ (see Subsec. 2.2). Consider now the equation $\widetilde{f}(z) = z$, to be compared with the equation for the QP energies, Eq. (60). The two solutions of this equation are $z_1 = 1$ and $z_2 = 2$, which are both real-valued. However, z_1 coincides with the branch point (Subsec. 2.1) of $\widetilde{f}(z)$ in the finite part of the complex z-plane. We further observe that $\partial\widetilde{f}(z)/\partial z$ diverges as $z \to z_1$. This complication may also occur while solving $\widetilde{\widetilde{E}}_s(z) = z$ (i.e. the solution may lie on the boundary of the region of analyticity of $\widetilde{\widetilde{E}}_s(z)$). For this reason it is important to establish the radius of convergence of the series through which $\widetilde{\widetilde{E}}_s(z)$ is calculated. As a matter of course, any solution outside this radius is false.

The consequence of the above-discussed possibility is that not all singular points of $\widetilde{G}(z)$ (or those of its associated functions, such as the spectral function) can be identified with energies of QPs (see in particular Footnote 51).

6.3. *Quasi-particles in homogeneous systems*

In the wave-vector representation (see Appendix A) for the non-interacting GF holds

$$\widetilde{G}_0(k;z) = \frac{\hbar}{z - \varepsilon_k^0}\,, \tag{72}$$

where

$$\varepsilon_k^0 := \frac{\hbar^2}{2m_e}k^2 \tag{73}$$

stands for the non-interacting-electron energy at $\mathbf{k}$. From the Dyson equation, Eq. (38), it thus follows that

$$\widetilde{G}(k;z) = \frac{\hbar}{z - [\varepsilon_k^0 + \hbar\widetilde{\Sigma}(k;z)]}\,. \tag{74}$$

Hence $\widetilde{E}_s(z)$, now denoted by $\widetilde{E}_k(z)$, is defined as

$$\widetilde{E}_k(z) := \varepsilon_k^0 + \hbar\widetilde{\Sigma}(k;z)\,. \tag{75}$$

As we have demonstrated earlier (Subsec. 5.1), for $|z| \to \infty$, $\widetilde{\Sigma}(k;z) \sim \Sigma^{HF}(k)$, the Hartree–Fock SE.[37] The exact form of this SE is unknown, but through

[37] For translation-invariant systems, the contribution of the Hartree part of the self-energy $\Sigma^H(k)$ (see Eq. (37)) to $\Sigma^{HF}(k)$ is infinite but is cancelled against equally infinite contribution due to interaction of electrons with the positively-charged uniform background. Hence, here $\Sigma^{HF}(k)$ and $\Sigma_s^{HF}(k)$ are identical with $\Sigma^F(k)$ and $\Sigma_s^F(k)$, respectively.

approximating the GS wavefunction by a single Slater determinant, one obtains the following form (Ashcroft and Mermin 1981, p. 334)

$$\Sigma_{\rm s}^{HF}(k) = -\frac{2e^2}{\pi\hbar} k_F \mathcal{F}(k/k_F)\,, \tag{76}$$

where

$$\mathcal{F}(x) := \frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right|. \tag{77}$$

This function decreases monotonically from 1 at $x = 0$, to 0 as $x \to \infty$, while $\mathcal{F}(1) = 1/2$. Above the subscript s indicates the underlying single-Slater-determinant approximation. In order to draw attention to the possibility that $\Sigma_{\rm s}^{HF}(k)$ may substantially deviate from the exact $\Sigma^{HF}(k)$, we point out that the pair-correlation function $g(r)$ (see Subsec. 8.8) as calculated in terms of a single Slater determinant of plane waves, non-negligibly departs from that calculated using a correlated GS wavefunction. For instance $g_{\rm s}(r)$ (i.e., $g(r)$ within the single-Slater-determinant approximation scheme) approaches 1/2 as $r \to 0$ (Glick and Ferrell 1959, Ueda 1961, March, Young and Sampanthar 1967, p. 12), whereas $g(r \to 0)$, depending on the value of electron density, can (due to the electron-electron repulsion) be substantially smaller than 1/2 (Ueda 1961, Singwi, Tosi, Land and Sjölander 1968, Singwi, Sjölander, Tosi and Land 1970). From the point of view of the many-body perturbation expansion, Σ^{HF} and $\Sigma_{\rm s}^{HF}$ differ in that the former is evaluated in terms of G, while the latter in terms of G_0.

Luttinger (1961) has shown that, as $\varepsilon \to \varepsilon_F$ [this result had been suggested earlier by Hugenholtz (1957, p. 544) and DuBois (1959b, p. 51)],[38]

$$\Sigma''(k;\varepsilon) \sim \mp\alpha_k(\varepsilon - \varepsilon_F)^2\,, \quad \varepsilon \gtrless \varepsilon_F\,, \quad (\text{with} \quad \alpha_k \geq 0)\,. \tag{78}$$

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[38] The result in Eq. (78) is, except for change of some symbols, *exactly* that presented in the work by Luttinger (1961). For the following reason, this result is somewhat inconsistent with our assertions: Whereas in the present work we distinguish between μ, μ_N ($\equiv \varepsilon_F$) and μ_{N+1} (see Subsec. 4.2), with $\mu_N < \mu < \mu_{N+1}$, in Luttinger's work, on account of the thermodynamic limit, the quantities μ_N and μ_{N+1} are identified with μ. According to our considerations, $\widetilde{\Sigma}(z)$ is real-valued and analytic in the *open* interval (μ_N, μ_{N+1}), whereas according to Luttinger's *no* such open interval exists. If we were consistent, then we had written (in what follows $\eta \downarrow 0$) : $\widetilde{\Sigma}''(k;\varepsilon) \equiv \Sigma''(k;\varepsilon) \equiv 0$ for $\varepsilon \in (\mu_N, \mu_{N+1})$; $\widetilde{\Sigma}''(k;\varepsilon + i\eta) \equiv \Sigma''(k;\varepsilon) \sim -\alpha_k(\varepsilon - \mu_{N+1})^2$ for $\varepsilon \geq \mu_{N+1}$; $\widetilde{\Sigma}''(k;\varepsilon - i\eta) \equiv \Sigma''(k;\varepsilon) \sim +\alpha_k(\varepsilon - \mu_N)^2$ for $\varepsilon \leq \mu_N$.

Employing this, the following *asymptotic* result, for small values of $|\varepsilon-\varepsilon_F|$, can be obtained from the first of the Kramers-Kronig-type relations in Eq. (50):

$$\Sigma'(k;\varepsilon) \sim \Sigma(k;\varepsilon_F) + \beta_k(\varepsilon-\varepsilon_F)\,, \quad (\text{with } \beta_k \leq 0)\,, \tag{79}$$

where

$$\Sigma(k;\varepsilon_F) \equiv \Sigma^{HF}(k) + \Sigma^{C}(k;\varepsilon_F)\,, \tag{80}$$

with Σ^C the "correlation part" (as opposed to the "exchange part", i.e. Σ^{HF}) of the SE operator. Perhaps partly due to Eqs. (78) and (79), a large body of the literature on the subject known to the present author invokes the suggestion that $\widetilde{\Sigma}(z)$ were analytic for z in the vicinity of $z=\varepsilon_F$. This is not the case, however. This can be seen in the following two alternative ways. First, the very fact that $z=\varepsilon_F$ is a branch point of $\widetilde{\Sigma}(z)$ implies that at $z=\varepsilon_F$ we must have to do with a *non-isolated* singularity (Subsecs. 2.1 and 2.2), from which it moreover follows that neither a Taylor series expansion nor even a Laurent series expansion can give a correct description of $\widetilde{\Sigma}(z)$ around this point (see Subsec. 2.3). Second, through explicit calculation of the next-to-leading-order term (that is the term following the one presented in Eq. (79)) in the asymptotic expansion for $\Sigma'(\varepsilon)$, for $|\varepsilon-\varepsilon_F| \to 0$, one directly observes that this term involves $(\varepsilon-\varepsilon_F)^2 \ln|\varepsilon-\varepsilon_F|$.[39] This logarithmic term underlines our above statement.

Let us now consider some of the consequences of the *asymptotic* expressions exposed above. Consider the equation for the QP energies on the real axis (see Eqs. (60) and (75)). We have $E_k(\varepsilon)=\varepsilon$, where, following Eqs. (78) and (79) for $\varepsilon \to \varepsilon_F$, $E_k(\varepsilon) \sim \varepsilon_k^0 + \hbar\{\Sigma(k;\varepsilon_F) + \beta_k(\varepsilon-\varepsilon_F) \mp i\alpha_k(\varepsilon-\varepsilon_F)^2\}$, when $\varepsilon \gtrless \varepsilon_F$. It can readily be verified that this asymptotic equation has a (real-valued) solution only if $\varepsilon = \varepsilon_k^0 + \hbar\Sigma(k;\varepsilon_F) = \varepsilon_F$. The second of the latter equalities, namely

$$\varepsilon_k^0 + \hbar\Sigma(k;\varepsilon_F) = \varepsilon_F\,, \tag{81}$$

is the equation defining the Fermi surface (Galitskii and Migdal 1958, Luttinger 1960, Eqs. (6) and (94) herein).[40] In analogy with the non-interacting theory,

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[39] Notice the logarithm function in $\int dx x^n/(a+bx) = \{\sum_{j=0}^{n-1}(-a/b)^j x^{n-j}/(n-j) + (-a/b)^n \ln|a+bx|\}/b$, for $n \geq 1$ (Gradshteyn and Ryzhik 1980, p. 58).

[40] Note that the definition of the Fermi surface involves Σ, whereas that of Z_{k_F} (see Footnotes 34 and 51) a *derivative* of Σ. Evidently, therefore, one can have a Fermi surface even when $Z_{k_F}=0$.

in which ε_k^0 plays the role of the energy of a "quasi-particle", and for which $\varepsilon_k^0 < \varepsilon_F^0$, with

$$\varepsilon_F^0 := \frac{\hbar^2}{2m_e} k_F^2 \tag{82}$$

the free-electron Fermi energy, defines the *interior* of the Fermi sea, we define the *interior* of the interacting Fermi sea as those regions of the momentum space where the LHS of Eq. (81) is less than the RHS (Luttinger 1960).

The isotropy of the problem at hand implies that the interacting Fermi surface, like that of the free-electron system, is spherical. However, there is a difference that can fundamentally alter the topology of the interacting-electron Fermi surface. Contrary to ε_k^0 which is a *monotonically increasing* function of k, interaction effects can *in principle* render $\varepsilon_k^0 + \hbar\Sigma(k;\varepsilon_F)$ a non-monotonically-increasing function of k (see Subsec. 6.5, in particular Footnote 51). If so, then the Fermi surface may consist of concentric spheres (see Footnote 6 in Luttinger 1960), each two of which *in general* alternatively enclose regions where $\varepsilon_k^0 + \hbar\Sigma(k;\varepsilon_F) < \varepsilon_F$ and where $\varepsilon_k^0 + \hbar\Sigma(k;\varepsilon_F) > \varepsilon_F$ (see Fig. 6). This sequence of alternating Fermi surfaces will be broken if solutions k of Eq. (81),

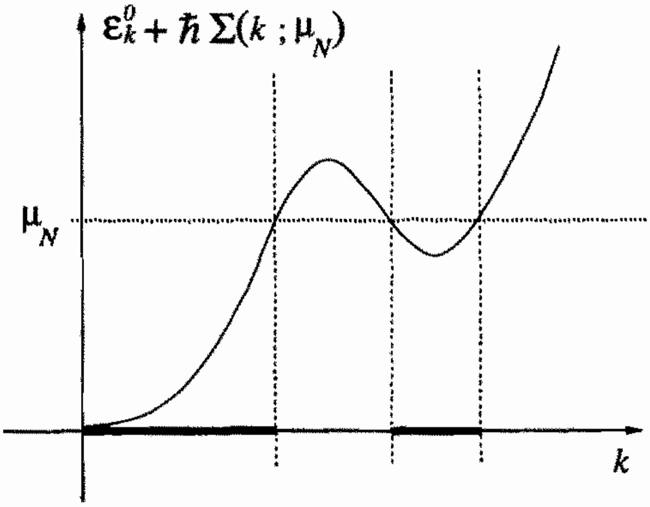

Fig. 6. A sketch of $\varepsilon_k^0 + \hbar\Sigma(k;\mu_N)$ — recall that $\mu_N \equiv \varepsilon_F$ and that $\mu_N < \mu < \mu_{N+1}$. Sections of the k-axis corresponding to $\varepsilon_k^0 + \hbar\Sigma(k;\mu_N) < \mu_N$, defining the *interior* of the Fermi sea, are indicated in bold. In the present case the Fermi sea consists of two concentric spherical parts. In a uniform system where $\varepsilon_k^0 \propto k^2$, the segmentation of the spherical Fermi sea of the non-interacting system (defined through $\varepsilon_k^0 < \mu_N^0$) is entirely due to the interaction effects. According to a theorem by Luttinger (1960) (Luttinger and Ward 1960), *volume* of the Fermi sea is not affected by interaction effects. We point out that contrary to the statement by Luttinger, a discontinuity in the momentum distribution function is *not* prerequisite to the existence of a Fermi surface, a fact that follows from Luttinger's (1960) own analysis; only it is necessary that $\Sigma(k;\mu_N)$ be real-valued for *all* k.

to which we shall refer as *zeros*, are of *even* order (here we restrict ourselves to the regular type of solutions), corresponding to a vanishing Fermi velocity (see Footnote 51); zeros k of higher than the second order are excluded, since such zeros will render $G(k;\varepsilon)$ non-integrable over the wave-vector space (see Eq. (74)). Further, at the largest k for which Eq. (81) is satisfied, it must hold $\partial\{\varepsilon_k^0 + \hbar\Sigma(k;\varepsilon_F)\}/\partial k \geq 0$. It is interesting to note that, whatever the arrangement of the Fermi surface, the total volume of its interior is exactly equal to the volume of the non-interacting Fermi sea (Luttinger 1960, Luttinger and Ward 1960). Through neglecting Σ^C in Eq. (80) *and* approximating $\Sigma^{HF}(k)$ by $\Sigma_s^{HF}(k)$ as presented in Eq. (76), the Fermi surface is seen to consist of a single surface, i.e. it retains the topology of the non-interacting-electron Fermi surface, whose radius is equal to k_F. It can readily be shown that the energy dispersion $\varepsilon_k^0 + \hbar\Sigma_s^{HF}(k)$ gives rise to a divergent Fermi velocity for the Landau QPs on the Fermi surface (Ashcroft and Mermin 1981, p. 337; see Footnote 51).

6.4. *Fermi versus non-Fermi liquid; a Luttinger's theorem revisited*

Now we should like to comment on Luttinger's result as presented in Eq. (78) above (Farid 1999a). To this end, it is appropriate that we first briefly describe the strategies and, most importantly, assumptions that have been instrumental to obtaining this result. Before proceeding we mention that our following considerations have direct bearing on three-dimensional homogeneous systems; Luttinger, in the work that we are about to discuss (Luttinger 1961), except for a brief remark restricts his considerations to such systems. In this remark it has been indicated how Eq. (78) fails to be valid in one-dimensional interacting systems (now referred to as "Luttinger-liquids" — Haldane 1981).[41]

Luttinger has obtained the result in Eq. (78) in the following manner: The proper SE operator (for a uniform-electron system) has been expanded in terms of skeleton diagrams (see Footnote 26). Describing the SE operator in terms of skeleton diagrams, implies a representation for the proper SE operator which *implicitly* (through the exact GF) depends upon the proper SE operator itself. After pointing out that $\Sigma(k;\varepsilon)$ owes its energy dependence to diagrams of second and higher order in the *bare* electron-electron interaction, Luttinger evaluates $\Sigma''(k;\varepsilon)$ for ε close to ε_F by considering in detail the contribution of a

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[41] For in-depth discussions of one-dimensional systems see Sólyom (1979) and Voit (1994); see also Subsec. 4.4 in Mahan (1981).

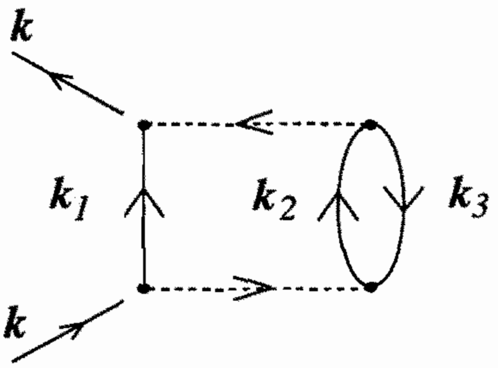

Fig. 7. A second-order proper self-energy diagram in terms of the bare particle-particle interaction (the broken lines) employed by Luttinger (1961). The solid lines stand for either G_0 or G, the single-particle Green functions pertaining to the non-interacting and interacting system, respectively. The external and internal wave-vectors, $\mathbf{k}$ and $\mathbf{k}_1$, $\mathbf{k}_2$ and $\mathbf{k}_3$, respectively, are shown. Due to the conservation of momentum, one of the internal wave-vectors, say $\mathbf{k}_3$, can be eliminated; $\mathbf{k}_3 = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}$.

second-order skeleton SE diagram (we have reproduced this diagram in Fig. 7). Of importance is that Luttinger proceeds by evaluating this contribution first in terms *not* of G but of G_0. Up to a multiplicative constant, this contribution turns out to be exactly that presented in Eq. (78). After this, under the *assumption* of general validity of Eq. (78),[42] Luttinger succeeds in demonstrating that the considered second-order SE skeleton diagram in terms of $G(\varepsilon)$ yields the same quadratic behaviour for $\Sigma''(k;\varepsilon)$. From this, Luttinger concludes that the leading-order contribution to $\Sigma''(k;\varepsilon)$, for ε approaching ε_F, does *not* depend on whether the skeleton SE diagrams are determined in terms of G or G_0. This simplifying result enables Luttinger to show that to all orders in the perturbation expansion, Eq. (78) is valid.[43]

Two general comments are in place. First, as is obvious from the above summary, Luttinger's result (Eq. (78)) has been obtained within the framework of the many-body PT. It has been pointed out (text preceeding Eq. (52) in the paper by Luttinger (1961); see also, e.g., the work by Mattuck (1976), p. 207) that Eq. (78) is therefore valid so long as the underlying many-body PT is valid. In other words, Eq. (78) may not be *a priori* universal since the many-body PT may break down.

[42] Roughly speaking, this *assumption* provides justification for replacing a Lorentzian by a Dirac δ-function (see Eqs. (68) and (69) in Luttinger 1961).

[43] This conclusion is arrived at by explicitly demonstrating that any skeleton SE diagram (in terms of G_0) of the 2nd and higher order in the *bare* electron-electron interaction makes a contribution to $\Sigma''(k;\varepsilon)$ which is proportional to $(\varepsilon - \varepsilon_F)^{2m}$ where $m \geq 1$.

The problem of the break-down of the zero-temperature ($T = 0$) many-body PT, in particular in homogeneous systems, has been addressed by Kohn and Luttinger (1960) and subsequently by Luttinger and Ward (1960), following the observation that *in general* the GS total energy as obtained from the $T \to 0$ limit of the perturbation expansion for the grand potential (Bloch and De Dominicis 1958) involves non-vanishing contributions that are identically vanishing within the framework of the zero-temperature many-body PT for the GS total energy (Goldstone 1957).[44] Kohn and Luttinger have shown that up to the second order of the PT, the two many-body PTs are identical for homogeneous systems (with spherical Fermi surfaces) of fermions of spin less than or equal to 1/2 (see Footnote 10 in the work by Luttinger and Ward (1960)). This result has subsequently been shown to be valid to all orders of the PT by Luttinger and Ward (1960). Since in the present work we are dealing with either spin-less Fermions or spin-compensated systems of spin-1/2 particles, we shall therefore not encounter a break-down of the perturbation expansion.[45] We point out that the unusual (i.e. non-Fermi-liquid-like) behaviour of the high-T_c compounds in their *normal* states has been associated with the low-lying excitations of these compounds forming a Luttinger liquid (Anderson 1990, 1991, 1992, 1993) — as opposed to a Fermi liquid —, and this in turn has been ascribed to the break-down of the many-body PT as applied (Engelbrecht and Randeria 1990, 1991) to these systems. We shall not explicitly touch upon this problem here.[46]

Second, the expansion concerning $\Sigma''(k;\varepsilon)$, for $\varepsilon \to \varepsilon_F$, of which the leading-order term we have presented in Eq. (78), *cannot* be a Taylor expansion with some non-vanishing radius of convergence, since ε_F is a (non-isolated) singular point (Subsec. 2.1) of $\widetilde{\Sigma}(k;z)$. Rather it is an asymptotic expansion (see Subsec. 2.3). The logarithmic corrections (Nozières 1964, p. 93) to the results in Eqs. (78) and (79) — see text following Eq. (80) above — make the validity of this statement evident.

Now we present a number of remarks on the technical aspects of Luttinger's work. First, the second-order diagram chosen by Luttinger (reproduced in

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[44] The diagrams corresponding to these non-vanishing contributions are referred to as "anomalous" diagrams. These have vanishing contributions for finite systems, however.

[45] Except that for sufficiently low electron densities, where the charge density of the non-interacting GS is uniform in contrast to that of the interacting system which is a Wigner crystal. In this regime of densities, the PT based upon a translation-invariant state naturally breaks down.

[46] Nonetheless, some elements of our present analyses are relevant to the on-going discussions on this subject.

Fig. 7) is in fact divergent for such long-range interaction functions as the Coulomb one. This is because both of the interaction lines in this diagram transfer the same amount of wave-vector, $\mathbf{k} - \mathbf{k}_1$. Since in three dimensions $v_c(k) \propto k^{-2}$, the integral over $\mathbf{k}_1$ diverges for vanishingly small $\|\mathbf{k} - \mathbf{k}_1\|$; by choosing the origin at $\mathbf{k}$, in the spherical-polar coordinate system (k_1, ϕ, θ) we have $d^3k_1 = dk_1 d\phi d\theta \; k_1^2 \sin(\theta)$, from which it is seen that in principle only poles of at most second order can be integrated over. Although the divergence of the second-order diagram adopted by Luttinger cancels by the contributions of a set of equally singular higher-order, random-phase approximation (RPA), diagrams (see, e.g., Pines and Nozières 1966, pp. 300–304, Mattuck 1976, pp. 185–192), it may be rightly questioned whether properties valid for the individual terms (e.g. $\propto (\varepsilon - \varepsilon_F)^2$) in such a highly singular infinite series necessarily survive the infinite summation. In this connection we mention that for series that are convergent, but not *absolutely* convergent, the sum depends on the order of summation (Whittaker and Watson 1927, pp. 18 and 25). Further, for series which are not *uniformly* convergent, the analytic properties of the sum may not coincide with any of those of the individual terms in the series (Whittaker and Watson 1927, pp. 91 and 92, Titchmarsh 1939, pp. 95–98). As for the problem under consideration, since a series whose terms are not finite cannot be absolutely or uniformly convergent (leaving aside that any finite sum of such a series is devoid of meaning), it is by no means clear whether the result in Eq. (78) can be of general validity for, say, the Coulomb systems.[47]

The divergent SE terms to which we have referred above, are those which involve at least two *bare* Coulomb interaction lines which carry the same wave-vector. Those diagrams that are attached through *two* bare interaction lines to the proper SE diagrams are *by definition* polarisation diagrams (Hubbard 1957, Fetter and Walecka 1971, p. 110). Since by conservation of wave-vector these two interaction lines *must* carry the same amount of wave-vector, it follows that all proper SE diagrams that contain *polarisation insertions* are therefore divergent (see Mattuck 1976, p. 188).

[47] It has been shown (Fukuyama, Narikiyo and Hasegawa, 1991; Fukuyama, Hasegawa and Narikiyo, 1991) that for the two-dimensional Hubbard model, within the t-matrix approximation (whose validity, in principle, is restricted to the low-density limit), $\Sigma''(k_F; \varepsilon + i\eta) \sim' (\varepsilon - \varepsilon_F)^2 \ln|\varepsilon - \varepsilon_F|$, as $\varepsilon \to \varepsilon_F$, with $\eta \downarrow 0$, which still signifies a Fermi-liquid behaviour (see Footnote 4). This logarithmic modification with respect to $(\varepsilon - \varepsilon_F)^2$, which has been known from the earlier works by Hodges, Smith and Wilkins (1971) and Bloom (1975), signifies the fact that *even* for short-range interactions it is not a safe procedure to draw conclusions with regard to $\Sigma''(k; \varepsilon)$ from the behaviour of the individual terms in a perturbation series expansion of $\Sigma(k; \varepsilon)$; for this to be a safe procedure, it is required that the *uniformity* of convergence of the latter series be ascertained (see Titchmarsh (1939), p. 95).

If we now analyse the proper SE diagrams in terms of the dynamic screened interaction function W (such analysis must then discard all proper SE diagrams that involve polarisation insertions — otherwise certain processes are multiply counted),[48] we readily observe that even in the lowest order of the perturbation expansion (see Subsec. 9), the behaviour of $\Sigma''(k;\varepsilon)$, in particular for $\varepsilon \to \varepsilon_F$, crucially depends on the charge-neutral excitation spectrum (as distinct from the single-particle, i.e. charged, excitation spectrum, which is contained in G) of the *interacting* system. Determination of this excitation spectrum, which is contained in the dynamic density-density correlation function $\chi(\varepsilon)$ (see Sec. 8 and in particular the closing paragraph of Subsec. 9.4), is as intractable a task as that of the single-particle excitation spectrum.[49]

6.5. *Breakdown of the many-body perturbation theory?*

In addition to the above, there is a technical aspect associated with the evaluation of $\Sigma''(k;\varepsilon)$ corresponding to the second-order diagram dealt with explicitly by Luttinger (see Fig. 7) that we find worth mentioning and commenting on. Conservation of wave-vector (or momentum) implies that of the three *internal* wave-vectors $\mathbf{k}_1$, $\mathbf{k}_2$ and $\mathbf{k}_3$, one is fully fixed by the other two; we have namely $\mathbf{k}_3 = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}$. Mathematically, this restriction follows from the fact that for the matrix element of the Coulomb potential (see Eq. (57) in the work by Luttinger (1961)) $(\mathbf{k},\mathbf{k}_3|v_c|\mathbf{k}_1,\mathbf{k}_2) = v_c(\mathbf{k}-\mathbf{k}_1)\delta_{\mathbf{k}-\mathbf{k}_1,\mathbf{k}_2-\mathbf{k}_3}$ holds. This implies that of the three 3-wave-vector integrals the one over, e.g., $\mathbf{k}_3$ can be eliminated. If one proceeds in this way, then the subsequent algebra becomes quite

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[48] In uniform systems (more generally, in all systems without a gap in their single-particle excitation spectrum — i.e. in systems with a Fermi surface) the static screened interaction function is shorter-ranged than the bare Coulomb interaction. Within the approximate Thomas-Fermi theory of screening, the static screened interaction is exponentially short-ranged (Fetter and Walecka 1971, pp. 175–178; Ashcroft and Mermin 1981, pp. 340–342), $W(\|\mathbf{r}-\mathbf{r}'\|;0) \propto \exp(-k_{TF}\|\mathbf{r}-\mathbf{r}'\|)/\|\mathbf{r}-\mathbf{r}'\|$, where k_{TF} stands for the Thomas-Fermi wavenumber; for metallic densities k_{TF}^{-1} ranges between 7.5 and 13.0 Å. This renders $W(k;0)$ finite for $k \to 0$. More accurate calculation, within the random-phase approximation (RPA), yields however a power-law decay for large $\|\mathbf{r}-\mathbf{r}'\|$: $W(\|\mathbf{r}-\mathbf{r}'\|;0) \sim' \cos(2k_F\|\mathbf{r}-\mathbf{r}'\|)/\|\mathbf{r}-\mathbf{r}'\|^3$ (Fetter and Walecka 1971, pp. 178 and 179; Ashcroft and Mermin 1981, p. 343), to be compared with $v_c(\mathbf{r}-\mathbf{r}') \propto 1/\|\mathbf{r}-\mathbf{r}'\|$. This is sufficient to rendering $W(k;0)$ finite for $k \to 0$; recall that $W(k;0) = \epsilon^{-1}(k;0)v_c(k)$, where $\epsilon(k;\varepsilon)$ stands for the dynamic dielectric response function (Subsec. 7.5), and that within the RPA (see Eq. (5.65) in Pines and Nozières (1966)), $\epsilon(k;0) \sim k_{TF}^2/k^2$, as $k \to 0$; with $v_c(k) \propto 1/k^2$, it is readily seen that indeed $W(k;0)$ is finite for $k \to 0$.

[49] Whereas $\Sigma''(\varepsilon)$ is a measure for the density of the excited *interacting* $N \pm 1$-states, $\chi''(\varepsilon)$ — see Eq. (112) — is a measure for the density of the excited *interacting* N-particle states.

tedious. Luttinger, in evaluating $\Sigma''(k;\varepsilon)$ corresponding to the diagram in Fig. 7 in terms of G_0, proceeds by transforming the wave-vector integrals over $\mathbf{k}_1$, $\mathbf{k}_2$ and $\mathbf{k}_3$ to those over the single-particle energies of the non-interacting problem $\varepsilon^0_{k_1}$, $\varepsilon^0_{k_2}$ and $\varepsilon^0_{k_3}$.[50] From Eq. (73) and the above expression for $\mathbf{k}_3$ it is readily seen that $\varepsilon^0_{k_3} = \varepsilon^0_{k_1} + \varepsilon^0_{k_2} + \varepsilon^0_k + (\hbar^2/m_e)\{\mathbf{k}_1 \cdot \mathbf{k}_2 - \mathbf{k} \cdot \mathbf{k}_1 - \mathbf{k} \cdot \mathbf{k}_2\}$. From this it is clear that in spatial dimensions higher than one, the *orientational* freedom of $\mathbf{k}_1$ and $\mathbf{k}_2$ with respect to each other as well as $\mathbf{k}$ permits independent variation of $\varepsilon^0_{k_3}$ alongside independent variations of $\varepsilon^0_{k_1}$ and $\varepsilon^0_{k_2}$ over non-vanishing intervals, in spite of the fact that $\mathbf{k}_3$ is completely fixed by $\mathbf{k}_1$ and $\mathbf{k}_2$. It is due to this possibility of *independent* variations in $\varepsilon^0_{k_j}$'s over non-vanishing intervals that for systems extending over more than one spatial dimension, Eq. (78) can hold — here, as far as contribution of the diagram in Fig. 7 in terms of G_0 is concerned.

Let us now in evaluating the contribution of the diagram in Fig. 7 in terms of G follow Luttinger in all respects. The QP energies being ε_k, following Luttinger, we will have to transform the integrals over wave-vectors $\mathbf{k}_1$, $\mathbf{k}_2$ and $\mathbf{k}_3$ by those over ε_{k_1}, ε_{k_2} and ε_{k_3},[51] to be compared with those over $\varepsilon^0_{k_j}$,

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[50] In the spherical polar coordinate system (k,ϕ,θ) we have $d^3k = k^2 \sin(\theta) dk d\phi d\theta$. With ε^0_k as given in Eq. (73), it follows that $d^3k \equiv \frac{1}{2}(2m_e/\hbar^2)^{3/2} \sqrt{\varepsilon^0_k} \sin(\theta) d\varepsilon^0_k d\phi d\theta$. Thus $d^3k \propto d\varepsilon^0_k$.

[51] Following Eqs. (60) and (75), ε_k is to satisfy $\varepsilon_k = \varepsilon^0_k + \hbar\Sigma(k;\varepsilon_k)$. As discussed in Sec. 6, for such ε_k to exist it is necessary that $\mu_N \le \varepsilon_k \le \mu_{N+1}$. In the present case only ε_{k_j}'s close to $\mu_N \equiv \varepsilon_F$ play a role. Therefore, leaving aside problems with regard to the differentiability of the functions involved, one can easily solve ε_k from the above equation to linear order in $(k - k_F)$ — such solution is of nature asymptotic. With $\varepsilon_k = \varepsilon_F + \partial\varepsilon_k/\partial k|_{k=k_F}(k-k_F) + \mathcal{O}\left((k-k_F)^2\right)$, some simple algebra yields $\partial\varepsilon_k/\partial k|_{k=k_F} = Z_{k_F}\partial\{\varepsilon^0_k + \hbar\Sigma(k;\varepsilon_F)\}/\partial k|_{k=k_F}$ where $Z_{k_F} := \left(1 - \hbar\partial\Sigma(k_F;\varepsilon)/\partial\varepsilon|_{\varepsilon=\varepsilon_F}\right)^{-1}$ — see Subsec. 6.6. In view of our discussions and remarks in Subsecs. 6.1 and 6.2, it is possible that $Z_{k_F} \equiv g_{k_F}$ (see Eq. (71)) may be vanishing, in which case one observes that to linear order in $(k - k_F)$, ε_k is a *constant* (unless $\partial\Sigma(k;\varepsilon_F)/\partial k \to \infty$ for $k \to k_F$ — see however further on). This behaviour of ε_k is fundamentally different from that of ε^0_k, for which holds $\varepsilon^0_k = \varepsilon^0_{k_F} + (\hbar^2 k_F/m_e)(k-k_F) + (\hbar^2/[2m_e])(k-k_F)^2$. For the effective mass m^*_e of the quasi-particle with energy ε_k at $k = k_F$ we have $m^*_e := \hbar^2 k_F/(\partial\varepsilon_k/\partial k|_{k=k_F})$, so that a vanishing $\partial\varepsilon_k/\partial k|_{k=k_F}$ would imply a diverging effective mass. However, one must be aware of the fact that this divergence merely signals the breakdown of the notion of quasi-particles on the Fermi surface (see Subsec. 6.2). Since for the Fermi velocity of the quasi-particle with energy ε_k at $k = k_F$ we have $v_F := \hbar^{-1}\partial\varepsilon_k/\partial k|_{k=k_F} \equiv \hbar k_F/m^*_e$, the above expansion for ε_k can alternatively be written as $\varepsilon_k = \varepsilon_F + \hbar v_F(k-k_F) + \mathcal{O}\left((k-k_F)^2\right)$. It is the linearised version of this expression that is invariably used for describing the behaviour of $G(k;\varepsilon)$ close to the Fermi surface (see, e.g., Migdal 1957, Nozières 1964, p. 93). Now let both $\partial\Sigma(k_F;\varepsilon)/\partial\varepsilon$ and

with $j = 1, 2, 3$. Now unless we make an explicit assumption concerning the dependence of ε_k upon k, such as for instance $\varepsilon_k = \hbar^2 k^2/[2m_e^*]$, with m_e^* the renormalised mass of the QPs (see Footnote 51), it is not possible to ascertain whether ε_{k_3}, with $\mathbf{k}_3 = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}$, can arbitrarily — i.e. independent of variations in ε_{k_1} and ε_{k_2} —, be varied over some finite interval (i.e. similar to what is the case for $\varepsilon_{k_3}^0$). If in a certain circumstance this is not the case, or range of variation in ε_{k_3} is infinitesimally smaller than ranges of variation in ε_{k_1} and ε_{k_2} (taking into account the requirement of the conservation of energy), for $\varepsilon \downarrow \varepsilon_F$ we may then have $\Sigma''(\varepsilon) \sim' (\varepsilon - \varepsilon_F)^{1+\gamma}$ where $\gamma \in [0, 1)$. We observe that Luttinger's derivation of Eq. (78) in a way implicitly excludes "non-Fermi-liquid" behaviour.[52] In other words, barring all possible problems associated with the derivation of Eq. (78) from the proper SE diagrams in terms of the *bare* Coulomb interaction (which we have discussed above), it is not incorrect to state that the result in Eq. (78) constitutes a possible *self-consistent* result, but by no means the only result that can be derived within the framework of the many-body PT. This implies that observation of non-Fermi-liquid behaviour in the low-energy (or low-temperature) properties of a homogeneous interacting system does not necessarily entail the breakdown of the many-body PT.

$\partial\Sigma(k;\varepsilon_F)/\partial k$ be unbounded for $\varepsilon = \varepsilon_F$ and $k = k_F$, respectively. Although *formally* the above expression for $\partial\varepsilon_k/\partial k|_{k=k_F}$ may be used to obtain $v_F = -\hbar^{-1}\, \partial\Sigma(k;\varepsilon_F)/\partial k|_{k=k_F}/ \partial\Sigma(k_F;\varepsilon)/\partial\varepsilon|_{\varepsilon=\varepsilon_F}$ (which may or may not be finite), it should be evident that in doing so one is neglecting the possibility that for, e.g., $k \downarrow k_F$ it may be the case that, for instance, $\Sigma(k;\varepsilon_F) \sim \Sigma(k_F;\varepsilon_F) + \alpha(k-k_F)^\sigma$, with $\sigma \in (0,1)$ (recall that a function's *asymptotic* series may not be *uniform* — see Subsec. 2.3); one is equally neglecting the possibility that for $\varepsilon \downarrow \varepsilon_F$ it may happen that, for instance, $\Sigma(k_F;\varepsilon) \sim \Sigma(k_F;\varepsilon_F) + \beta\,(\varepsilon-\varepsilon_F) + \gamma(\varepsilon-\varepsilon_F)\ln(\varepsilon-\varepsilon_F)$. In such cases, v_F is clearly an altogether unsubstantial quantity and *cannot* be defined: In order to define v_F, it is necessary that for $k \to k_F$ one can write $\varepsilon_k = \varepsilon_F + \hbar v_F(k-k_F) + R(k)$, where $R(k) = o(k-k_F)$; although $R(k)$ may be a singular function of k at $k = k_F$, the property $R(k) = o(k - k_F)$ ensures existence of a finite first derivative of ε_k at $k = k_F$. At least one of the above typical asymptotic expressions for $\Sigma(k;\varepsilon_F)$ and $\Sigma(k_F;\varepsilon)$ is sufficient to cause that *no* such $R(k)$ exists and therefore render $\varepsilon_k = \varepsilon_F + \hbar v_F(k - k_F) + R(k)$ devoid of any meaning. In the proof of Luttinger's theorem no account has been taken of the above possibilities, which cannot be *a priori* ruled out. Finally, it is important to point out that Galitskii's (1958) results, for the real and imaginary parts of ε_k close to $k = k_F$, obtained through solving the Galitskii integral equations, yielding a linear behaviour for the former and a quadratic one for the latter (linear and quadratic in $(k - k_F)$), are explicitly determined for short-range fermion-fermion interactions (see Farid 1999a).

[52] Using the Kramers-Kronig relation in Eq. (48), it can be shown that $\Sigma''(\varepsilon) \sim' |\varepsilon - \varepsilon_F|^\sigma$, as $\varepsilon \to \varepsilon_F$, implies the following for $\Sigma'(\varepsilon) - \Sigma(\varepsilon_F)$: (1) $\sim' (\varepsilon - \varepsilon_F)$ when $1 < \sigma \leq 2$; (2) $\sim' (\varepsilon - \varepsilon_F)\ln|\varepsilon - \varepsilon_F|$ when $\sigma = 1$ ("marginal Fermi-liquid" behaviour); (3) $\sim' (\varepsilon - \varepsilon_F)^\sigma$ when $0 < \sigma < 1$.

6.6. *Momentum-distribution function; a Migdal's theorem revisited*

In view of the above discussions it is instructive that we consider a well-known result due to Migdal (1957); this result has also been obtained, through a somewhat alternative approach, by Luttinger (1960).

Migdal (1957) first establishes that the momentum-distribution function $\mathsf{n}(k)$ (to be precise, here "wave-number distribution function") in the GS of a uniform electron system,

$$\mathsf{n}(k) := \langle \Psi_{N,0} | \widehat{a}_k^\dagger \widehat{a}_k | \Psi_{N,0} \rangle \, , \tag{83}$$

is directly related to the hole part of the GF, G^h (see Eq. (10)) in the momentum representation. From this, upon deformation of the contour of the energy integration along the real axis into the complex energy plane, Migdal obtains[53]

$$\mathsf{n}(k) = \frac{1}{\hbar} \int_C \frac{dz}{2\pi i} \widetilde{G}(k;z) \, , \tag{84}$$

where C denotes the contour as depicted in Fig. 8. Now Migdal states that for k infinitesimally less than k_F, denoted by k_F^-, $\widetilde{G}(k;z)$ has a pole, with an infinitesimal imaginary part (due to $\Sigma''(k;\varepsilon)$ — see Eq. (78)), enclosed by contour C in Fig. 8, and that through increasing k to $k_F^+ (k_F^+ > k_F)$, the imaginary part of the mentioned pole changes sign, upon which the pertinent pole leaves the interior of C.[54] Aside from this *singular* part (the singularity being, according to Migdal, a simple pole), the GF has also a *regular* or *incoherent* part which does not contribute to $\mathsf{n}(k_F^-) - \mathsf{n}(k_F^+)$ — because of it being *regular*. Thus it follows that (see Eqs. (79))

$$\mathsf{n}(k_F^-) - \mathsf{n}(k_F^+) = Z_{k_F} := (1 - \hbar \beta_{k_F})^{-1} \, , \tag{85}$$

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[53] The notation here is ours — Migdal does not employ $\widetilde{G}(k;z)$. Further, the convention adopted by Migdal for G differs from ours by a minus sign.

[54] Strict application of the notation of the present work would demand that we denoted k_F^- by k_F, the latter via Eq. (81) corresponding to $\varepsilon_F \equiv \mu_N$. Thus we would only need to define k_F^+ corresponding to $\varepsilon_F^+ \equiv \mu_{N+1}$. As we have mentioned earlier (see Subsec. 4.2 and Footnote 38), in our case μ is interior to an *open*, albeit infinitesimal, interval on the ε-axis where both $\widetilde{G}(k;z)$ and $\widetilde{\Sigma}(k;z)$ are analytic.

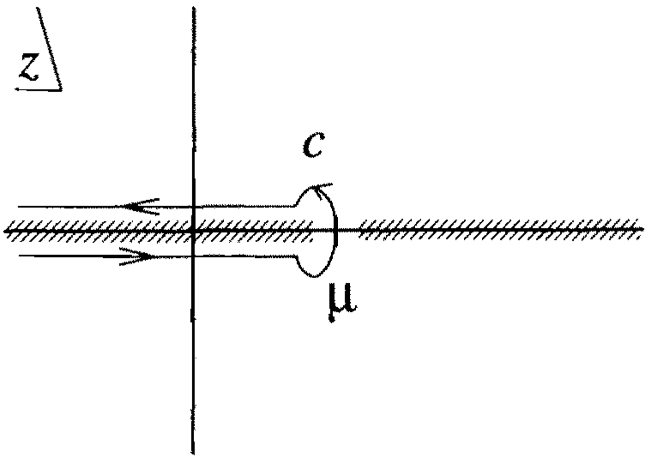

Fig. 8. Contour of integration employed in the proof of the Migdal theorem concerning the discontinuity of the wavevector (or momentum) distribution function $\mathsf{n}(k)$ at $k = k_F$ and its relation to the quasi-particle weight on the Fermi surface, Z_{k_F}.

where $Z_{k_F} \equiv g_{k_F}$, as defined in Eq. (71). This result is correct in as far as Eq. (78), and therefore Eq. (79), is correct (see Subsec. 6.5).[55]

We now restate the arguments put forward by Migdal in the mathematical language of the present work (see Footnote 54). The singularity of $\widetilde{G}(k_F;z)$ at $z = \varepsilon_F (\equiv \mu_N)$ and of $\widetilde{G}(k_F^+;z)$ at $z = \varepsilon_F^+ (\equiv \mu_{N+1})$ [see following paragraph] are *not* isolated so that neither $z = \varepsilon_F$ nor $z = \varepsilon_F^+$ can be a *pole*; they are branch points (see Subsec. 2.1) of $\widetilde{G}(k_F;z)$ and $\widetilde{G}(k_F^+;z)$, respectively. What renders Migdal's result nevertheless correct is the specific form of the asymptotic result in Eq. (78), so that as far as the integral over C is concerned, the singularity of $\widetilde{G}(k_F;z)$ at $z = \varepsilon_F$ (see Eqs. (74) and (81)) can be *thought of* as being a pole circumscribed by C. The situation would be the same if instead of the result in Eq. (78), we would for instance have $\Sigma''(k;\varepsilon) \sim \mp\alpha_k|\varepsilon - \varepsilon_F|^{1+\gamma}$ with $\gamma > 0$, for $\varepsilon \gtrless \varepsilon_F$ (see Footnote 38). For $\gamma = 0$ and $-1 < \gamma < 0$, $\mathsf{n}(k_F^-)$ would admit a vanishing contribution from the singularity of $\widetilde{G}(k_F;z)$ at $z = \varepsilon_F$ (see Footnote 52); this case corresponds to marginal Fermi-liquid and one-dimensional interacting systems, known as "Luttinger liquids" (Footnote 5 in the work by Luttinger (1961), Luttinger (1963), Mattis and Lieb (1965), Haldane (1981), Voit (1994) — see Subsec. 6.2 and Footnote 51), respectiviely.

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[55] For Z_{k_F} calculated for electrons interacting via the Coulomb potential see Hedin (1965), Rice (1965) and Hedin and Lundqvist (1969) and for $\mathsf{n}(k_F^-) - \mathsf{n}(k_F^+)$ calculated for fermions interacting via a repulsive hard-core potential see Galitskii (1958) and Belyakov (1961). For $\mathsf{n}(k)$ calculated within the RPA see Daniel and Vosko (1960) and for an accurate model for this function see Farid, Heine, Engel and Robertson (1993).

Further, according to Eq. (78), $\Sigma''(k;\varepsilon)$ is vanishing for $\varepsilon = \varepsilon_F$ and $\varepsilon = \varepsilon_F^+$ (see Footnote 38), so that contrary to the statement by Migdal (see text following Eq. (84)), the imaginary part of the "pole" of $\widetilde{G}(k;z)$ at $z = \varepsilon_F$ *cannot* change sign upon changing k from $k_F (\equiv k_F^-)$ to k_F^+. Using our strict conventions (see in particular Footnotes 38 and 54 — see also Sec. 6), $\widetilde{G}(k;z)$ is everywhere analytic with the exception of some points and intervals of the real energy axis. Thus even without reliance on the asymptotic result in Eq. (78), it is evident that whatever the nature of the singularity of $\widetilde{G}(k;z)$ that contributes to Eq. (85), it can be nowhere but on the real energy axis. This singularity is the solution of Eq. (81) (see Eq. (74)). One observes that rather than the imaginary part of the singular point of $\widetilde{G}(k;z)$ changing sign for k displaced from k_F to k_F^+, Eq. (81), which is satisfied for $k = k_F$, ceases to be satisfied for $k = k_F^+$ and therefore $\widetilde{G}(k_F^+;\varepsilon_F)$ is *bounded*; the equation fulfilled by $k = k_F^+$ is $\varepsilon_k^0 + \hbar\Sigma(k;\varepsilon_F^+) = \varepsilon_F^+$. Evidently, $\varepsilon_F^+ \equiv \mu_{N+1}$, which is the point where $\widetilde{G}(k_F^+;z)$ is *unbounded*, is located in the exterior of the region enclosed by the contour C in Fig. 8 (see also Figs. 3 and 4) and therefore has no contribution to $\mathsf{n}(k_F^+)$.

The conclusion that may be drawn from the above considerations is that through a careful process of analytic continuation, and making clear distinction between various branches of many-valued functions (classified as "physical" and "non-physical"), there arises no need for invoking such *ad hoc* assumption as "change in sign of $\Sigma''(k;\varepsilon)$" upon changing k from k_F^- to k_F^+ (see Farid 1999a).

6.7. *Some comments concerning solutions of the quasi-particle equation*

In Subsec. 6.1 we considered solution of the QP equation $\mathcal{E}_s(z) = z$; under the assumption that this equation possesses only one solution (which in general is located on the non-physical RS), we have denoted this by z_s. As we have further mentioned, unless z_s be real-valued, it cannot be considered as corresponding to some stationary one-particle eigenstate of the fully interacting Hamiltonian $\widehat{H}$; for a complex z_s, the corresponding QP describes a superposition of a macroscopically large number of degenerate and almost degenerate stationary eigenstates of $\widehat{H}$, so that it cannot be asserted that "the state" corresponding to z_s would have evolved, in the course of the adiabatic switching-on of the perturbation $\widehat{H} - \widehat{H}_0$, from a single eigenstate of the non-interacting Hamiltonian H_0 corresponding to energy ε_s^0 (notice the subscript s, which we have chosen to be the same subscript as in z_s). We recall the popular statement, that the Landau theory of Fermi liquids relies upon the implicit assumption that eigenstates of $\widehat{H}$ stand in a one-to-one correspondence with those of $\widehat{H}_0$ (Landau 1957a). This assumption is justified (in an asymptotic sense) *a posteriori* by Eq. (78) for the *low-energy* excitations of the many-electron system; this clarifies the reason for the applicability of the Landau theory (if it is applicable at all) to describing properties corresponding to low-laying excited states of interacting systems.

Another point of some relevance is the following. Suppose that by *some* means $\mathcal{E}_s(z) = z$ has been solved and that the solution z_s happens to be close to ε_s^0, in particular that $|\mathrm{Im}(z_s)| \ll |\mathrm{Re}(z_s)|$. In such an event, one might wish to obtain the "physical" counterpart of z_s, i.e. ε_s (this is not necessarily the same energy that features in the Lehmann representation for $G(\varepsilon)$ in Eq. (11)), through *iteratively* (DuBois 1959a, pp. 208–210) solving the first equation in Eq. (69), adopting a finite-order Taylor expansion for $E_s(\varepsilon) := \widetilde{E}_s(\varepsilon + \mathrm{sgn}[\varepsilon - \mu]i\eta)$ (see Eq. (65)) around $\varepsilon = \varepsilon_s^{(i)}$, with $i = 0, 1, \ldots$, where $\varepsilon_s^{(0)} \equiv \varepsilon_s^0$. Here the requirement for "iteration" arises from the non-linearity of $E_s(\varepsilon)$ [around $\varepsilon_s^{(i)}$], leading to the general property that $\varepsilon_s^{(i+1)} \neq \varepsilon_s^{(i)}$ for $i \geq 1$. Let us for simplicity make use of a first-order Taylor expansion. The *linear* equation thus obtained has the following solution

$$\begin{aligned}\varepsilon_s^{(i+1)} &= \frac{\varepsilon_s^0 + \mathrm{Re}(E_s(\varepsilon_s^{(i)})) - \mathrm{Re}(E_s^{\prime}(\varepsilon_s^{(i)}))\varepsilon_s^{(i)}}{1 - \mathrm{Re}(E_s^{\prime}(\varepsilon_s^{(i)}))} \\ &\approx \varepsilon_s^0 + \mathrm{Re}(E_s(\varepsilon_s^{(i)})) + \mathrm{Re}(E_s(\varepsilon_s^{(i)}))\mathrm{Re}(E_s^{\prime}(\varepsilon_s^{(i)}))\,, \qquad (86)\end{aligned}$$

where $E_s^{\prime}(\varepsilon) := \partial E_s(\varepsilon)/\partial\varepsilon$. In what follows we assume ε_s^0 to be very close to ε_s so that $\varepsilon_s^{(i+1)}$ with $i = 0$ is to a high degree of accuracy equal the desired real-valued solution.[56]

For uniform systems of electrons, $\widetilde{E}_s(z) \leftrightarrow \varepsilon_k^0 + \hbar\widetilde{\Sigma}(k; z)$ (see Eq. (75)) so that $\widetilde{E}_s^{\prime}(z) \leftrightarrow \hbar\partial\widetilde{\Sigma}(k; z)/\partial z$. For these systems, DuBois (1959a, pp. 208–210; see also DuBois (1959b, pp. 66 and 67)) has shown that derivatives like $\partial\widetilde{\Sigma}^{(m)}(k; z)/\partial z \equiv \partial\widetilde{E}_k^{(m)}(z)/\partial z$ in the above expression, with $\widetilde{\Sigma}^{(m)}(k; z)$ denoting the total contribution of the mth-order SE diagrams (including both skeleton and *non-skeleton* diagrams) in the perturbation expansion for $\widetilde{\Sigma}(k; z)$ in terms of the dynamically-screened electron-electron interaction, gives rise to

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[56] That this procedure can produce *real-valued* solutions, is *not* at variance with our earlier statement that $\widetilde{E}_s(z) = z$ *in general* has *no* solution. This is because taking the real part of a complex function is *not* an analytic process.

(a) (b)

Fig. 9. Two self-energy (SE) diagrams in terms of the single-particle Green function G_0 of some "non-interacting" Hamiltonian (solid directed line) and the dynamic screened interaction function W (wavy line). Diagram (b) is *not* skeleton but contributes to the SE operator due to use of G_0. The derivative with respect to the external energy parameter ε of diagram (a) gives rise to a contribution that partly cancels contribution of diagram (b) to $\Sigma(\varepsilon)$. When $\Sigma(\varepsilon)$ is approximated by a finite-order perturbation series, $\partial\Sigma(\varepsilon)/\partial\varepsilon$ involves incompletely-compensated contributions.

contributions that cancel some terms in $\widetilde{\Sigma}(k;z)$ originating from $\widetilde{\Sigma}^{(m+1)}(z)$.[57] Thus for $i = 0$, there is a (partial) cancellation between $\mathrm{Re}(E_s(\varepsilon_s^0))$ and $\mathrm{Re}(E_s(\varepsilon_s^0))\mathrm{Re}(E_s^I(\varepsilon_s^0))$ in the second expression on the RHS of Eq. (86). As an example, the derivative with respect to ε of diagram (a) in Fig. 9 gives rise to a contribution that counters some contribution due to diagram (b) in the same Figure.

Two conclusions may be drawn from the above considerations:[58]

First, when $\Sigma(\varepsilon)$ has been obtained through a *finite-order* perturbation expansion in terms of some G_0, derivatives of $\Sigma(\varepsilon)$ involve contributions that in the exact theory do *not* contribute, due to the above-mentioned cancellation. Since such cancellation is *not* complete when a finite-order perturbation expansion for $\Sigma(\varepsilon)$ has been employed, it is consequently appropriate to use $\varepsilon_s \approx \varepsilon_s^0 + \mathrm{Re}(E_s(\varepsilon_s^0))$ and neglect the term involving $\mathrm{Re}(E_s^I(\varepsilon_s^0))$ on the RHS of Eq. (86) — (Rice 1965, second paragraph on p. 111). For a specific example of such cancellation, concerning low-temperature heat capacity of a degenerate uniform-electron system, see DuBois (1959b, pp. 66 and 67).

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[57] It can be directly verified that $\partial\langle s|\widetilde{G}_0(z)|s'\rangle/\partial z = -\hbar\langle s|\widetilde{G}_0(z)\widetilde{G}_0(z)|s'\rangle$. We have, moreover, $\widetilde{E}_s(z) \approx {}_0\langle s|H_0|s\rangle_0 + {}_0\langle s|\widetilde{\Sigma}(z)|s\rangle_0$. Here $\{|s\rangle\}$ denotes any (complete) set of one-electron states, and $\{|s\rangle_0\}$ that of normalised eigenstates of H_0.

[58] Lack of space prevents us from doing due justice to the subject matter, so that here we essentially quote other authors.

Second, in a perturbative calculation of the GF, the SE diagrams and the vertex-function diagrams (see Subsec. 7.5) should be concomitant or "corresponding"; this on account of certain cancellation property (Mahan 1994).[59] Self-energy diagrams have two external points and the vertex-function diagrams three (see Subsec. 7.5). Concomitant SE and vertex diagrams give rise to contributions in, say, the polarisation function that largely cancel (Mahan 1994). The criteria put forward by Baym and Kadanoff (1961) and Baym (1962) on the one hand, and the Ward (1950) identities (Nozières and Luttinger 1962, Nozières 1964, Mahan 1992) on the other, provide means by which to select out sets of vertex-function diagrams that are concomitaut with a given set of SE diagrams.

7. Determination of The Single-Particle Green Function

In this Section we review several methods for calculating the GF of an interacting system. We give our main attention to the many-body perturbation theory.

7.1. *Exact approach*

The single-particle Green function $G(\mathbf{r}t,\mathbf{r}'t')$ can *in principle* be determined from its defining equation, Eq. (8). This implies, amongst others, knowledge of the GS wavefunction, so that this approach becomes impracticable for systems with even a moderate number of electrons. For completeness, for describing the time-dependence of the field operators in the Heisenberg picture, here use should be made of the Trotter formula (Negele and Orland 1988, p. 337).[60] In doing so, since $G(\mathbf{r}t,\mathbf{r}'t')$ is a function of $t-t'$, the time argument of one of the field operators can be held fixed.

7.2. *Equation-of-motion approach and truncation of hierarchy*

The equation-of-motion (EOM) for G directly follows from the EOM for the annihilation field operator (or its Hermitian conjugate, the creation field

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[59] We draw attention of the reader to misprints in (Mahan 1994). For instance, on pp. 346 and 347 of this work, the Hubbard G(k) within the LDA is mentioned to be equal to $-K_{xc}$ while in reality this G(k) is equal to $-K_{xc}/v_c(k)$. Further, we should like to mention that the screened interaction W_5 suggested in (Mahan 1994) is incorrect on physical grounds — see (Farid 1997a).

[60] For a realisation of this approach (in combination with a Monte-Carlo technique for integration) for applications to systems involving coupled boson-fermion fields see Blankenbecler, Scalapino, and Sugar (1981).

operator) in the Heisenberg picture, namely (Fetter and Walecka 1971, p. 59),

$$i\hbar\frac{\partial\widehat{\psi}_H(\mathbf{r}t)}{\partial t} = [\widehat{\psi}_H(\mathbf{r}t), \widehat{H}]_-\,, \tag{87}$$

where $[\ ,\ ]_-$ stands for the commutation operation. Because of the two-body (Coulomb) interaction, involving *four* field operators (see Eq. (5)), the EOM for G is *not* closed but hierarchical: it involves the two-particle GF (see, e.g., the work by Kadanoff and Baym (1962), Ch. 3). For the same reason, the EOM for the n-particle GF involves the $(n+1)$-particle GF. Thus in practice solving the EOM for G is only feasible if at certain level the hierarchy is broken, which amounts to suppression of an infinite class of interaction processes (these of course may not be significant processes for the physical properties of interest). It is important to point out that truncation of the hierarchy of the GFs in an arbitrary fashion may lead to violation of the gauge invariance and of all or some of the conservation laws. Baym and Kadanoff (1961) and Baym (1962) have analysed this subject in considerable detail.

The EOM for the GF even at the crudest level of truncation of the hierarchy of the GFs is *non-linear*, implying a multiplicity of solutions. A major difficulty in dealing with such non-linear EOM is that of singling out the correct solution from amongst these. We shall return to this subject in Subsubsec. 7.4.1.

7.3. *Conserving approximations*

Baym and Kadanoff (1961), amongst other things, present *sufficient* conditions to be met by the approximate two-particle GF in order for the truncated hierarchy of the GFs (see Subsec. 7.2) to constitute a gauge invariant and conserving formalism (conditions (A) and (B) in the paper by Baym and Kadanoff (1961), p. 290). We shall not touch upon the details of these criteria here, but only mention that according to Baym (1962), these are satisfied when the SE operator is the functional derivative with respect to G of a constant functional Φ, i.e. when $\Sigma(\mathbf{r}t,\mathbf{r}'t') \equiv \delta\Phi/\delta G(\mathbf{r}'t',\mathbf{r}t)$ — this is, therefore, a statement of a *sufficient* condition for an approximate framework to be gauge invariant and conserving. A scheme based upon some chosen functional Φ is referred to as a "Φ-drivable conserving approximation".[61] For applications of this approximation see, e.g., works by Bickers, Scalapino and White (1989), Bickers and

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[61] In general a Φ-derivable approximation is *not* invariant under the so-called *exchange* or *crossing* symmetry. For definition and details see the work by Bickers and White (1991).

Scalapino (1989), Bickers and White (1991), Serene and Hess (1991), Dahm and Tewordt (1995a,b), Micnas, *et al.* (1995) and Dahm, Manske and Tewordt (1997).

7.4. *Many-body perturbation theory, and its breakdown*

The GF can in principle be determined through application of the many-body PT (for technical aspects see, e.g., Fetter and Walecka 1971, Negele and Orland 1988). Elsewhere (Farid 1997a, 1999b) we have in some detail discussed the problems from which the many-body PT can suffer. Therefore here we shall be brief and mention that a perturbation expansion *can* fail because (i) the perturbation series may diverge as a whole; (ii) some of the terms contributing to the perturbation series may be divergent; (iii) after having summed *all* terms of the series — barring possible difficulties due to problems (i) and (ii) —, the outcome may be unrelated to the sought-after single-particle GF ("bogus convergence").

7.4.1. *In defence of the many-body perturbation theory*

Problem (i) can be understood by analogy with the following simple example. Consider $S_n(x) := 1 + x + \cdots + x^n$. For $n \to \infty$ this series is absolutely convergent only when $|x| < 1$ (it is, however, conditionally convergent for $x < 1$, in the sense of being Borel summable (Whittaker and Watson 1927, pp. 154 and 155, Lauwerier 1977, pp. 45–50, Negele and Orland 1988, pp. 373–376)),[62] and it diverges otherwise. Thus although $S_n(x)$ for $n \to \infty$ is *formally* a series expansion for $(1 - x)^{-1}$, it has no validity when x lies outside some specified domain. In the same way, a many-body perturbation expansion for G in terms of some "reasonable" non-interacting Green function G_0 can become invalid when interaction, or perturbation, becomes too "strong".[63]

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[62] For other summation techniques (like Cesàro's and that by Riesz) see (Whittaker and Watson 1927, pp. 154–156).

[63] There is a subtlety involved here. Contrary to an ordinary series, a many-body perturbation series involves products of matrix elements of the "perturbation" with respect to the initial, intermediate and final many-electron states. Hence the "strength" of the perturbation is not solely determined by the "perturbation" itself — in the second example in Subsubsec. 7.4.3 we shall see that, for a particular model, irrespective of the magnitude of the coupling constant λ of perturbation, but as long as $\lambda > 0$, the Rayleigh-Schrödinger perturbation series yields the *exact* GS total energy. In some cases (such as that concerning a uniform system of electrons), the perturbation Hamiltonian may involve a multiplicative dimensionless parameter through which the "strength" of the perturbation can be regulated. However, the perturbation series in powers of such parameter may *not* be convergent, but

Problem (ii) arises quite generally. However, for the so-called *re-normalisable* field theories (Collins 1984), divergent terms can be made harmless through partial summation of specified classes of perturbation terms. In other words, divergent terms in such field theories have always counter-terms. For the theory adopted here, as described by $\widehat{H}$ in Eqs. (2)–(5), the *possible* singular terms in the perturbation expansion for G arise from certain polarisation terms (diagrammatically represented by the so-called "loop" diagrams — see Subsecs. 6.4 and 8.4): due to the long range of the *bare* Coulomb interaction, in the momentum space this interaction is singular in the long-wavelength limit, so that the mentioned terms *may* involve divergent momentum integrals corresponding to "zero"-momentum-transfer polarisation processes ("infra-red" divergence). Now we can distinguish between two types of systems: those that do *not* have gap in the low-energy part of their single-particle excitation spectrum (such as metals) and those that *do have* a gap in this spectrum (such as semiconductors and insulators). In the former systems, where one encounters divergent momentum integrals, the partial summation over the polarisation diagrams results in a *screened* electron-electron interaction function which is shorter-ranged than the bare Coulomb interaction (see Footnote 48) and, in addition, is energy dependent. This screened interaction renders divergent momentum integrals convergent. Therefore through a partial summation over the polarisation diagrams — which amounts to expressing the perturbation series in terms of the dynamic screened interaction function, as opposed to the static bare Coulomb interaction function —, the theory is renormalised. In the latter case, existence of a fundamental gap in the single-particle excitation spectrum renders contributions of all polarisation diagrams finite.[64] We emphasise that

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asymptotic and divergent (Subsec. 2.3), no matter how small the parameter — see Subsubsec. 7.4.2. A divergence of this type may be circumvented by performing the perturbation expansion in terms of a "non-interacting" Hamiltonian that *implicitly* depends upon the interaction, so that the resulting perturbation series is not merely a power series in the perturbation parameter. See Footnote 69.

[64] This can be understood by recalling the fact that in applying perturbation theory to a manifold of degenerate states, it is required first to construct a suitable linear combination of these states, for otherwise a perturbation, no matter how weak, gives rise to divergent contributions. For states corresponding to non-degenerate energy levels, no similar measure need be taken. In elementary quantum mechanics these subjects are dealt with under the headings of "degenerate perturbation theory" and "perturbation theory", respectively. In the present case, systems with a Fermi surface (whose "occupied" energy levels are infinitesimally below μ [i.e. at μ_N and lower] and "un-occupied" energy levels infinitesimally above μ [i.e. at μ_{N+1} and higher]) present us with a situation comparable with one where "degenerate perturbation theory" needs to be applied ("perturbation" here being the electron-electron

"renormaliseability" and "convergence" of a perturbation expansion are two entirely distinct issues: A re-normalisable series is *not* necessarily convergent. We can therefore conclude that in our case problem (ii) is not a fundamental problem.

Problem (iii) is a most serious one in that it does not show up in the form of a divergence, and can therefore go undetected. The possibility of failure of the PT on this ground has been known since long (Kohn and Luttinger 1960, Luttinger and Ward 1960). Problem (iii) has its origin in the following. The many-body PT, in particular that for the single-particle Green function, with $\widehat{H}_0$ the "non-interacting" Hamiltonian and $\widehat{H}_1 := \widehat{H} - \widehat{H}_0$ the "perturbation" Hamiltonian, is based on the *assumption* that the GS of the interacting Hamiltonian $\widehat{H}$ (which we denote by $|\Psi_{N,0}\rangle$) is *adiabatically connected* with the GS of the non-interacting Hamiltonian $\widehat{H}_0$, $|\Phi_{N,0}\rangle$. By this it is meant that through an *adiabatic* transformation of $\widehat{H}_0$ into $\widehat{H}$, by means of increasing τ in $\widehat{H}_0 + \exp(-\eta|\tau|/\hbar)(\widehat{H} - \widehat{H}_0) =: \widehat{H}_\eta(\tau)$, with $\eta \downarrow 0$ (from there "adiabatic"), from $-\infty$ to 0, $|\Phi_{N,0}\rangle$ *adiabatically* converts into $|\Psi_{N,0}\rangle$ and, moreover, through further increasing τ from 0 to $+\infty$, $|\Psi_{N,0}\rangle$ goes over into a state which up to a trivial phase factor is identical with $|\Phi_{N,0}\rangle$. This *assumption* has its origin in a theorem due to Gell-Mann and Low (1951) which asserts that the process of "adiabatic switching-on" connects $|\Phi_{N,0}\rangle$ with *some* eigenstate of $\widehat{H}$ (see Fetter and Walecka 1971, pp. 61–64, Farid 1997a, 1999b). In other words, the validity of the many-body PT relies upon the assumption that in changing τ from $-\infty$ to 0, the GS of $\widehat{H}_\eta(\tau)$ either remains non-degenerate — as any level crossing at *some* intermediate $\tau \in (-\infty, 0)$ *may* lead to disconnection of $|\Psi_{N,0}\rangle$ from $|\Phi_{N,0}\rangle$ —, or in the event that there is some level-crossing at, say, at $\tau = \tau_1$, there is a subsequent level-crossing at $\tau = \tau_2$ (with $\tau_1 < \tau_2 < 0$) which restores the adiabatic connection between $|\Phi_{N,0}\rangle$ and $|\Psi_{N,0}\rangle$.

A direct consequence of the adiabatic disconnection of $|\Psi_{N,0}\rangle$ from $|\Phi_{N,0}\rangle$ can be easily appreciated by realising that the single-particle GF is the expectation value of $-i\mathcal{T}\{\widehat{\psi}_H(\mathbf{r}t)\widehat{\psi}_H^\dagger(\mathbf{r}'t')\}$ with respect to the *ground state* of $\widehat{H}$ in the Heisenberg picture (see Eq. (8) above), so that G, calculated perturbatively, is accordingly the expectation value with respect to whatever many-body state (as indicated, not necessarily the GS) that has been evolved from

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Coulomb interaction). The mentioned partial summation over the polarisation diagrams differs, however, from application of the "degenerate perturbation theory" in that it amounts to a *redefinition* of the "perturbation" ("bare interaction" → "screened interaction") at the expense of eliminating the polarisation processes.

$|\Phi_{N,0}\rangle$ through the process of "adiabatic switching-on" of $\widehat{H}-\widehat{H}_0$. In this way, despite the possible convergence of the many-body perturbation series for G, the calculated function is unrelated to the actual G for which the perturbation series has been set up (see the second example in Subsubsec. 7.4.3).

In a way the above problem is related to that which arises in solving the non-linear EOM for G to which we have referred in Sec. 7.2. The connection is readily seen as follows: As mentioned above, the EOM for $G(\mathbf{r}t,\mathbf{r}'t')$ is obtained from that for $\widehat{\psi}(\mathbf{r}t)$. Here one multiplies both sides of the latter equation (Eq. (87)) by $\widehat{\psi}^{\dagger}(\mathbf{r}'t')$ and subsequently applies the time-ordering operator to the resulting equation. After some algebraic manipulations, one takes the expectation values of both sides of the thus-obtained *operator-valued* equation with respect to $|\Psi_{N,0}\rangle$, upon which the sought-after EOM for $G(\mathbf{r}t,\mathbf{r}'t')$ is obtained. Obviously, the only aspect in this equation that hints at it being the EOM for the single-particle GF is the mere *appearance* of the symbol "$G(\mathbf{r}t,\mathbf{r}'t')$" in it! Had we *bracketed* the mentioned *operator-valued* EOM for $-i\mathcal{T}\{\widehat{\psi}(\mathbf{r}t)\widehat{\psi}^{\dagger}(\mathbf{r}'t')\}$ between *any* normalised N-electron eigenstate of the number operator $\widehat{N}$, say, $|X_N\rangle$ (or, more generally, had we *bracketed* the mentioned operator-valued equation between $\langle Y_N|$ and $|X_N\rangle$ with $\langle Y_N|X_N\rangle \neq 0$), we had obtained a similar-looking EOM for $-i\langle X_N|\mathcal{T}\{\widehat{\psi}(\mathbf{r}t)\widehat{\psi}^{\dagger}(\mathbf{r}'t')\}|X_N\rangle/\langle X_N|X_N\rangle$ which is distinct from $G(\mathbf{r}t,\mathbf{r}'t')$, unless $|X_N\rangle \equiv |\Psi_{N,0}\rangle$. This implies that each of the multiplicity of solutions of the EOM for G may in fact correspond to one such amplitude. Assuming $|X_N\rangle$ to be, in addition, a simultaneous eigenstate[65] of $\widehat{H}$, we immediately observe how the possibility of adiabatic disconnection of the GS of $\widehat{H}_0$ from that of $\widehat{H}$, leading to the breakdown of the many-body PT for G, on the one hand and the multiplicity of the solutions of the EOM for G on the other, are closely related.

Problems (i) and (iii) can in principle be overcome through a suitable choice for the non-interacting Hamiltonian: one whose GS is "adiabatically connected" with the GS of $\widehat{H}$. In (Farid 1997a, 1999b) it has been shown that provided some specific condition(s) be satisfied (see further on), one such non-interacting Hamiltonian can even be explicitly calculated. Briefly, within the framework of the DFT appropriate to a specific system, one has to do with a well-specified set of GS properties that *uniquely* determine the many-body GS. For instance, for a system of spin-less fermions with non-degenerate GS, the GS is a *unique* functional of the GS charge density $n(\mathbf{r})$ (Hohenberg and Kohn

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[65] The adiabatic evolution of the GS of $\widehat{H}_0$ *always* results in an eigenstate of $\widehat{H}$ — see (Gell-Mann and Low 1951, Fetter and Walecka 1971, pp. 61 and 64, Farid 1997a).

1964). Now provided this n be *pure-state non-interacting v-representable* (see Footnote 7), it is, by definition, also the density of the non-degenerate GS of a *non-interacting* Hamiltonian, referred to as the Kohn-Sham (KS) Hamiltonian — named after Kohn and Sham (1965) who have originally put forward this Hamiltonian for systems of spin-compensated electrons with non-degenerate GSs. In (Farid 1997a,b) it has been shown that for any specific system whose relevant densities (such as the total electronic density, the spin-polarisation density, the total paramagnetic current density, etc.) are *pure-state* non-interacting v-representable, the many-body PT in terms of the pertinent KS Hamiltonian is unrestrictedly valid.[66] We can therefore conclude that problem (iii), within the just-mentioned limitation with regard to the pure-state non-interacting v-representability of the relevant densities, is *not* unsurmountable. It should be realised that since GSs of KS Hamiltonians yield the exact relevant (in the above-indicated sense) GS densities pertaining to the associated interacting systems, and since GSs of these systems are *unique* functionals of the mentioned densities (Hohenberg and Kohn 1964), it follows that KS Hamiltonians are appropriate for use, as "non-interacting" Hamiltonians, in the perturbation expansions concerning *all* (dynamic) GS correlation functions, and *not exclusively* for use in the perturbation expansion of the single-particle GF. In Sec. 8 we shall explicitly demonstrate the superiority of the perturbation expansion of the dynamic density-density correlation function in terms of the non-interacting GF pertaining to the KS Hamiltonian.[67] Computational results in (Farid 1997a,b), concerning some GS properties pertaining to spin-less fermions in a qnasi one-dimensional system and electrons with spin confined to a two-dimensional plane and exposed to an external magnetic field, demonstrate the extreme reliability as well as practicability of a many-body PT in terms of the relevant KS Hamiltonian. Description of the mentioned systems is known to be beyond the reach of a straight-forward many-body PT.

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[66] In (Negele and Orland 1988, p. 167) we read: "The ultimate conclusion, then, is that there is nothing fundamentally wrong with the zero-temperature [perturbation] theory. Rather, to do sensible physics, one must pick an intelligent choice for H_0 such that $|\Phi_0\rangle$ has the right symmetries and corresponds to the correct physical phase of the system, and such that $V = v - U$ [i.e., the perturbation] is sufficiently small to obtain reasonable convergence." In (Farid 1997a,b) it has been shown that the KS Hamiltonian qualifies as one such "intelligent choice for H_0."

[67] The permutation invariance of the square of a many-electron wavefunction implies that when the charge density pertaining to an eigenstate is converged, the wavefunction corresponding to it is also converged over the *entire* configuration space.

7.4.2. *Dyson's argument*

Here we draw attention to an argument put forward by Dyson (1952)[68] to the effect that in general perturbation series (in powers of the coupling constant of interaction) should be divergent asymptotic series (for definition see Subsec. 2.3). Although this may be the case in some circumstances, Simon (1970) has demonstrated the incorrectness of Dyson's argument in its generality. Aside from this, the following two observations have to be taken into account: (i) Divergent asymptotic series can be summed (by various summation techniques — see Subsec. 2.3), yielding functions that are analytic in specific sectors of the complex plane of the pertinent expansion parameter (here, a coupling-constant parameter); the divergence of these series is then seen to correspond to singularities of these analytic functions;[69] (ii) In practice, perturbation expansions are almost never carried out around the GS of the *truly non-interacting* Hamiltonian (take for instance the expansion around the GS of the KS Hamiltonian [whose use within the context of the many-body PT we have advocated in Subsubsec. 7.4.1], which takes account of the electron-electron interaction to infinite order). That is, in practice many-body perturbation series are almost never in powers of the coupling constant of the bare electron-electron interaction.

7.4.3. *Simon's argument; two counter examples*

According to Simon (1970), Dyson's (1952) arguments are based on two "folk theorems": (i) that analytic continuation of an eigenvalue in the complex plane

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[68] We have to emphasise, however, that Dyson (1952) has qualified his argument as follows: "The argument here presented is lacking in mathematical rigour and in physical precision. It is intended only to be suggestive, to serve as basis for further discussions." Nonetheless, this "argument" is frequently used in disregard to its apparent limitations.

[69] Consider the energy per electron, in Rydberg, of a uniform system of interacting electrons (Gell-Mann and Brueckner 1957, Pines and Nozières 1966, p. 304): $E_{N,0}/N = 2.21/\bar{r}_s^2 - 0.916/\bar{r}_s + 0.062\ln(\bar{r}_s) - 0.096 + a\bar{r}_s + b\bar{r}_s\ln(\bar{r}_s) + c\bar{r}_s^2 + \cdots$, where $\bar{r}_s := r_s/a_0$, with $r_s := (9\pi/4)^{1/3}/k_F$, the Wigner-Seitz radius, and $a_0 := \hbar^2/[m_e e^2]$ the Bohr radius (one thus observes that indeed $\bar{r}_s \propto e^2$, the electron-charge squared, i.e. the coupling constant of the electron-electron interaction). The first two terms in this expression are the *uncorrelated* kinetic and exchange energy, respectively, and the remaining terms account for the correlation energy. Were it not because of the terms involving $\ln(\bar{r}_s)$ (which has a branch point at $\bar{r}_s = 0$), the energy density of electrons had a second-order pole at $\bar{r}_s = 0$ on the complex $\bar{r}_s$-plane. Because of the terms involving $\ln(\bar{r}_s)$, one observes that $E_{N,0}/N$ *cannot* be described in terms of a Laurent series in $\bar{r}_s$. Nevertheless, the above expression for $E_{N,0}/N$ has been obtained from a perturbation series, involving infinite number of divergent terms. Compare with the asymptotic and divergent series in Subsec. 2.3, corresponding to the analytic function $z^{-1}\exp(1/z)\Gamma(0,1/z)$.

of the coupling constant of a theory (assuming a scalar coupling constant) should necessarily be an eigenvalue; (ii) that when a perturbation series converges, it does converge to the physically meaningful limit. Both of these assertions are in their generality false (Simon 1970). We point out that incorrectness of (ii), at least in general and in so far as the GF is concerned, should be manifest from our arguments presented in Subsubsec. 7.4.1 (under "Problem (iii)").

As for assertion (i), consider the following one-particle Hamiltonian corresponding to a one-dimensional systems (expressed in the Hartree atomic units):

$$\mathcal{H} := -\frac{1}{2}\frac{d^2}{dx^2} + \lambda x^4\,, \quad -\infty < x < \infty\,. \tag{88}$$

It is shown (Simon 1970) that for $\lambda > 0$, eigenvalues of this Hamiltonian are $\mathcal{E}_n(\lambda) := c_n \lambda^{1/3}$, with c_n independent of λ. Since $\widetilde{\mathcal{E}}_n(z) \equiv c_n z^{1/3}$ has third-order branch points (Subsec. 2.1) at $z = 0$ and $1/z = 0$, analytic continuation of $\widetilde{\mathcal{E}}_n(z)$ along a closed contour *encompassing* the origin, starting and returning to $z = \lambda_0 (> 0)$ yields a complex-valued $\widetilde{\mathcal{E}}_n(\lambda_0)$ (according to the conventions that we have adopted in the present work, this function should be denoted by $\widetilde{\widetilde{\mathcal{E}}}_n(\lambda_0)$), unless the contour has been traversed a multiple of three times. Clearly, a complex-valued $\widetilde{\mathcal{E}}_n(\lambda_0)$ *cannot* be an eigenvalue of a self-adjoint operator.

As for assertion (ii), consider the following hydrogen-like problem in three dimensions (expressed in the Hartree atomic units):

$$\mathcal{H} := -\frac{1}{2}\nabla^2 - \frac{\lambda}{r}\,, \quad r \geq 0\,, \tag{89}$$

where λ, when positive integer, plays the role of the atomic number Z. The eigenvalues of this problem for bound states, i.e. those corresponding to $\lambda > 0$, form the well-known Balmer series: $\mathcal{E}_n(\lambda) = c_n \lambda^2$, with $c_n := -1/[2n^2]$. According to the latter expression, $\mathcal{E}_n(\lambda)$ is negative for *all* real values of λ, implying bound states even for $\lambda < 0$, which is evidently erroneous. This false result belongs to the same class as the one that we have considered under (i) above. Now since $\mathcal{E}_n(\lambda)$ is a finite-order *polynomial* (explicitly, a second-order one) and therefore an analytic function of λ, the Rayleigh-Schrödinger perturbation expansion (March, Young and Sampanthar 1967, pp. 72–74) for, say, the GS energy (i.e. $\mathcal{E}_{n=1}(\lambda)$) — with the second term on the RHS of Eq. (89) playing the role of the "perturbation" — yields $-\lambda^2/2 \equiv \mathcal{E}_1(\lambda)$, irrespective of whether

$\lambda > 0$ or $\lambda \leq 0$ *and* irrespective of the magnitude of λ; the coefficients of λ^m, for $m = 0, 1$ and $m > 2$, are *all* identically vanishing, establishing an infinite number of exact sum-rules. Since $\mathcal{H}$ in Eq. (89) has no bound states for $\lambda < 0$, it immediately follows that for $\lambda < 0$ the perturbation series converges to a physically incorrect value ("bogus" convergence).

From the above example we can draw one important conclusion in support of our statement that PTs in terms of the appropriate KS Hamiltonians are unconditionally valid, provided the pertinent densities be pure-state non-interacting v-representable (see Subsec. 7.4.1). The GS density for one electron, $n_\lambda(r)$, corresponding to $\mathcal{H}$ in Eq. (89) is the square of the amplitude of the GS wavefunction. For $\lambda > 0$ we have $n_\lambda(r) := \psi_{0;\lambda}^2(r) \equiv \lambda^3 \exp(-2\lambda r)/\pi$. We immediately observe that whereas $\mathcal{E}_1(\lambda) \equiv -\lambda^2/2$ suggests a GS for $\lambda < 0$, incorporation of the knowledge with regard to $n_\lambda(r)$ in the application of the PT immediately informs us of the incorrectness of this inference, for the simple reason that the above $n_\lambda(r)$ becomes *trivial* for $\lambda = 0$ and *unbounded* for $\lambda < 0$. It follows that incorporation of information with regard to $n_\lambda(r)$ indeed prevents the above "bogus" convergence in the events $\lambda \leq 0$.

7.5. *Set of self-sufficicnt equations*

An elegant method for obtaining the single-particle GF without *explicit* reference to the many-body PT is based on the variation of a *local* time-dependent source term in the Hamiltonian that directly couples to the density of the particles (Schwinger 1951a, b, c, Anderson 1954, Matsubara 1955, Martin and Schwinger 1959, Kato, Kobayashi and Namiki 1960, Hedin 1965). Such a *local* source term, $\varphi(j)$, with j the short for $\mathbf{r}_j t_j$, is sufficient for the purpose of calculating the GF. This source term is an auxiliary function and is set equal to zero after the desired equations have been derived. Hedin (1965), through employing this approach has obtained the following set of four coupled equations, known as the Hedin equations:

$$P(1,2) = \frac{-2i}{\hbar} \int d(3)d(4)G(1,3)G(4,1^+)\Gamma(3,4;2)\,, \tag{90}$$

$$\Sigma(1,2) = \frac{i}{\hbar} \int d(3)d(4)G(1,3)W(4,1^+)\Gamma(3,2;4)\,, \tag{91}$$

$$W(1,2) = v_c(1,2) + \int d(3)d(4)v_c(1^+,3)P(3,4)W(4,2)\,, \tag{92}$$

$$\Gamma(1,2;3) = \delta(1,2)\delta(1,3) + \int d(4)d(5)d(7)\frac{\delta\Sigma(1,2)}{\delta G(4,5)} \times G(4,6)G(7,5)\Gamma(6,7;3)\,. \tag{93}$$

Here $t^+ \downarrow t$, $v_c(1,2) := v_c(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2)$ and $\delta(1,2) := \delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2)$. The functions P, W and Γ are the polarisation function, the dynamic screened interaction function and the vertex function, respectively. The pre-factor of 2 on the RHS of Eq. (90) is due to a trace over an internal spin degree of freedom of electrons (for spin-$\mathbf{s}$ particles, the pre-factor would be $2\mathbf{s} + 1$). These expressions are made complete through the Dyson equation in Eq. (38). The equation for W, first derived by Hubbard (1957) through application of the many-body perturbation theory, can equally be expressed in terms of the inverse of the dielectric function, ϵ^{-1}, as follows

$$W(1,2) = \int d(3)\epsilon^{-1}(1,3)v_c(3,2) \tag{94}$$

where

$$\epsilon^{-1}(1,2) = \delta(1,2) + \int d(3)v_c(1^+,3)\chi(3,2)\,, \tag{95}$$

with χ denoting the dynamic density-density correlation function,

$$\chi(\mathbf{r}t,\mathbf{r}'t') := \left.\frac{-2i\delta G(\mathbf{r}t,\mathbf{r}t^+;[\varphi])}{\delta\varphi(\mathbf{r}'t')}\right|_{\varphi=0} \equiv \frac{-2i}{\hbar}\langle\Psi_{N,0}|\mathcal{T}\{\widehat{\rho}_H(\mathbf{r}t)\widehat{\rho}_H(\mathbf{r}'t')\}|\Psi_{N,0}\rangle\,. \tag{96}$$

The pre-factors 2 on the RHS of Eq. (96) are due to a trace over the two spin states of an electron. In Eq. (96) $[\varphi]$ indicates that G is a functional of the external source term. In Eq. (96), $\widehat{\rho}_H(\mathbf{r}t)$ stands for the charge-fluctuation operator (with respect to the GS charge density $n(\mathbf{r})$) in the Heisenberg representation (see Eqs. (119) and (120) below)

$$\widehat{\rho}_H(\mathbf{r}t) := \widehat{\psi}_H^{\dagger}(\mathbf{r}t)\widehat{\psi}_H(\mathbf{r}t) - \frac{1}{2}n(\mathbf{r})\,. \tag{97}$$

Above, as in the defining expression for the GF in Eq. (8), $\mathcal{T}$ stands for the *fermion* time-ordering operator, although contrary to $\widehat{\psi}^{\dagger}$ and $\widehat{\psi}$, $\widehat{\rho}$ is a bosonic operator as it involves a product of an *even* number of fermionic field operators.

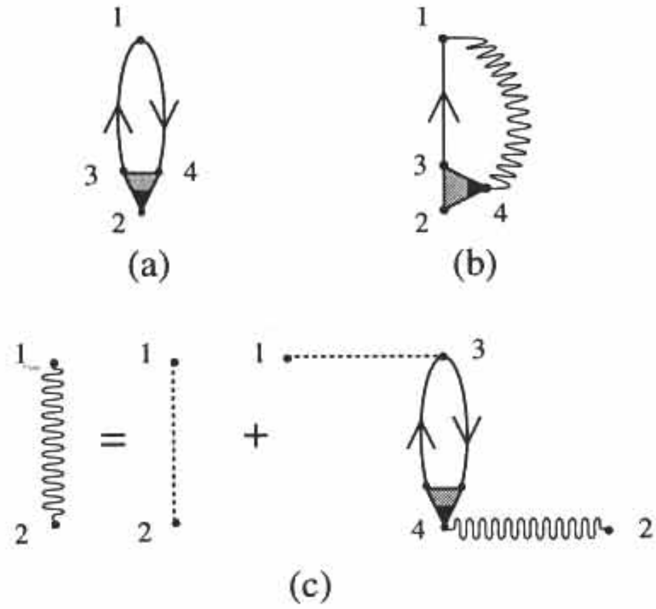

Fig. 10. (a) Diagrammatic representation of the polarisation function $P(1,2)$ and (b) of the self-energy operator $\Sigma(1,2)$ excluding the Hartree part $\Sigma^H(1,2)$. A solid line directed from j to i stands for $G(i,j)$ and a wavy line between j and i for $W(i,j)$ — owing to $W(\mathbf{r}',\mathbf{r};\varepsilon) = W(\mathbf{r},\mathbf{r}';\varepsilon)$ and $W(\mathbf{r},\mathbf{r}';-\epsilon) = W(\mathbf{r},\mathbf{r}';\epsilon)$, direction of this line is immaterial. In (c) the diagrammatic representation of the integral equation for $W(1,2)$ is given. The broken line between j and i represents $v_c(i,j) \equiv v_c(\mathbf{r}_i - \mathbf{r}_j)\delta(t_i - t_j)$ — direction of this line is also immaterial. The triangle in (a) whose coroners are numbered 3, 4 and 2 stands for the vertex function $\Gamma(3,4;2)$ — the first (second) argument can only be attached to a GF line which is directed from (towards) it, whereas the last argument (corresponding to the marked corner of the triangle) can only be attached to an interaction line. Note the different ways in which Γ enters in the diagrams for P and Σ.

We note in passing that the dielectric function ϵ, whose inverse is presented in Eq. (95), is one of a group of three functions that often are designated by the same name, namely "dielectric function" (Kleinman 1968). The function in Eq. (95) is more completely designated as the "electron-test-charge dielectric function" whose characteristic feature is that in it χ is pre-multiplied by the bare electron-electron interaction function v_c.

In Fig. 10 we present the diagrammatic representations for $P(1,2)$, $\Sigma(1,2)$ (excluding the Hartree part, Σ^H) and $W(1,2)$ in Eqs. (90), (91) and (92). The diagrammatic representation of the perturbation expansion for $\Gamma(1,2;3)$ in terms of G and W is presented in Fig. 11.

In closing this Section, we point out that a self-consistent solution G of Eqs. (90)–(93), supplemented by the Dyson equation, will suffer from the same type of problem that we have indicated in Subsec. 7.2 (see also the second half of Subsec. 7.4.1): the solution not being unique (due to the apparent

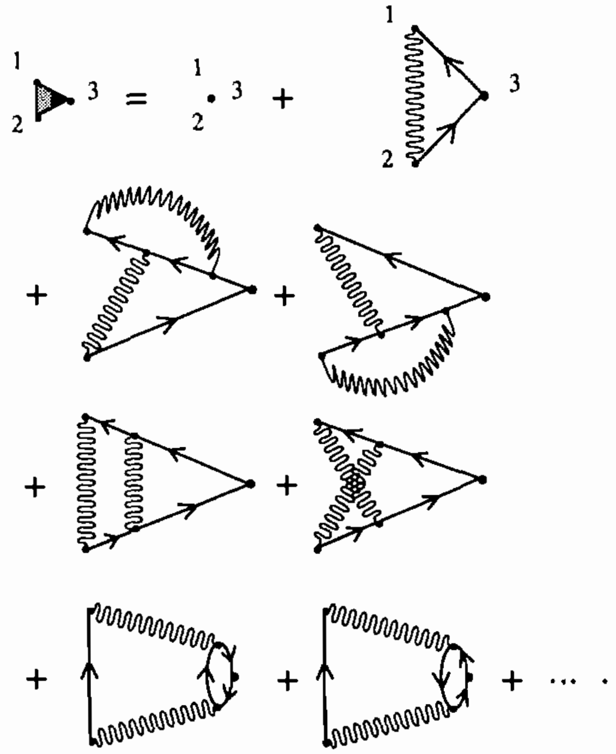

Fig. 11. Diagrammatic representation of the perturbation series expansion for $\Gamma(1,2;3)$ in terms of the single-particle Green function G (solid line) and the *dynamic* screened electron-electron interaction W (wavy line). Diagrams up to and including the second-order in W are shown. The solid dot directly following the equal sign stands for $\delta(1,2)\delta(1,3)$ where $\delta(i,j) \equiv \delta(\mathbf{r}_i - \mathbf{r}_j)\delta(t_i - t_j)$. Incorporation of *only* this contribution in the expression for P gives rise to the Random-Phase Approximation (RPA) for the polarisation function, and in the expression for Σ, to the dynamically-screened exchange, or GW, approximation for the self-energy operator.

non-linearity of the equations), one can obtain such solutious that are entirely unrelated to the actual G. To dispose of this problem, it is necessary that some subsidiary conditions (i.e., the "inequality constraints" defined in Subsec. 9.8) be imposed on the solution (such as the GS total energy corresponding to G — see Eq. (214) below —, be minimal).

7.6. *Two functional forms for thc self-energy operator, $\Sigma^{\{0\}}$ and $\Sigma^{\{1\}}$*

Traditionally, the SE operator Σ that, for instance, features in the Dyson equation $G = G_0 + G_0\Sigma G$ is defined under the assumption that the non-interacting Hamiltonian $\widehat{H}_0$, whose GF is G_0, does *not* in any way depend upon the electron-electron interaction v_c, that is $\widehat{H}_0$ is both explicitly *and* implicitly *independent* of v_c. Although such $\widehat{H}_0$ is in almost all cases of any interest a very poor starting point from the perspective of the PT, nevertheless it frees Σ from the ills of multiple definition in different texts. Thus, e.g., the electrostatic Hartree potential v_H is always accounted as being part of $\hbar\Sigma$. Now if, for instance, G_0 corresponds to a "non-interacting" Hamiltonian that incorporates the Hartree potential v_H, the appropriate Dyson equation should be denoted by $G = G_0 + G_0\Sigma_1 G$, where Σ_1 stands for $\Sigma - \hbar^{-1}v_H$. More generally, if $\widehat{H}_0$ besides v_H takes into account some other potentials, a local one v_L (such as the exchange-correlation potential v_{xc} that features in the "non-interacting" KS Hamiltonian — see Eq. (135) below) and a non-local one v_{NL} (such as the Fock part of the SE — see Eq. (37) above and Eq. (212) below), one has

$$\Sigma_1 := \Sigma - \frac{1}{\hbar}(v_H + v_L + v_{NL})\,. \tag{98}$$

It is evident that $\hbar\Sigma_1$ is nothing but the deviation of $\hbar\Sigma$ from the effective potential in H_0 that in some average way represents the electron-electron interaction. Since $\hbar^{-1}v_H$ *explicitly* occurs in the perturbation expansion for Σ, $(\Sigma - \hbar^{-1}v_H)$ is independent of v_H; we shall express this fact by enclosing $\Sigma - \hbar^{-1}v_H$ by a pair of parentheses. Further, since v_L and v_{NL} are supposed to be potentials contributing to H_0, it is necessary that $v_L + v_{NL}$ be Hermitian.

Let us for a moment leave aside problems related to the general invalidity of the many-body perturbation for an arbitrary choice for the "non-interacting" Hamiltonian (see Subsubsec. 7.4.1). From the structure of the perturbation series for Σ, as represented by the pertinent Feynman diagrams, it can readily be observed that Σ, and thus also Σ_1, is a *functional* of G_0; we denote this functional by $\Sigma^{\{0\}}[G_0]$. On the other hand, by restricting the set of perturbation diagrams for the SE operator to that of the skeleton diagrams (see Footnote 26), the SE is seen to be a functional of G, which we therefore denote by $\Sigma^{\{1\}}[G]$ (see Fig. 10(b) in conjunction with Fig. 11). Evideutly $\Sigma^{\{0\}}[F] \not\equiv \Sigma^{\{1\}}[F]$ for any function (or operator) F that functionally is equivalent with G_0 or G (i.e., in the $\mathbf{r}t$-representation, F is a function of *two* spatial variables $\mathbf{r}$ and $\mathbf{r}'$ and one time variable $t - t'$). These remarks apply to G, and, in the cases where $\widehat{H}_0$ is explicitly or implicitly dependent upon v_c, also to G_0. From this we draw two important conclusions: First, all functionals in Eqs. (90) — (93) are, in our just-introduced notation, those with superscript $\{1\}$. Second, the Σ_1 that we have introduced in Eq. (98), stands for either

$$(\Sigma^{\{1\}} - \hbar^{-1} v_H)[G] - \frac{1}{\hbar}(v_L + v_{NL}) =: \Sigma_1^{\{1\}}[G] \quad \text{or}$$

$$(\Sigma^{\{0\}} - \hbar^{-1} v_H)[G_0] - \frac{1}{\hbar}(v_L + v_{NL}) =: \Sigma_1^{\{0\}}[G_0] . \tag{99}$$

The distinction between $\Sigma_1^{\{0\}}[F]$ and $\Sigma_1^{\{1\}}[F]$ arises from the second and higher-order SE terms in the PT (see Sec. 9). By assuming $v_L \equiv v_{xc}$, with v_{xc} the *exact* exchange-correlation potential as defined within the framework of the DFT (see Eq. (132)), and $v_{NL} \equiv 0$, we have $v_H[G] \equiv v_H[G_0]$.

8. The Density–Density Correlation Function χ and the Polarisation Function P

For the time-Fourier transform of χ in Eq. (96), along the same lines as for the GF, one obtains the following Lehmann-type representation

$$\chi(\mathbf{r}, \mathbf{r}'; \varepsilon) = 2 \sum_s \varrho_s(\mathbf{r}) \varrho_s^*(\mathbf{r}') \left\{ \frac{1}{\varepsilon - e_s + i\eta} - \frac{1}{\varepsilon + e_s - i\eta} \right\} , \tag{100}$$

where (owing to $\langle \Psi_{N,0} | \Psi_{N,s} \rangle = \delta_{s,0}$)

$$\varrho_s(\mathbf{r}) := \begin{cases} 0, & \text{when } s = 0 , \\ \langle \Psi_{N,0} | \widehat{\psi}^\dagger(\mathbf{r}) \widehat{\psi}(\mathbf{r}) | \Psi_{N,s} \rangle , & \text{when } s \neq 0 , \end{cases} \tag{101}$$

and

$$e_s := E_{N,s} - E_{N,0} \geq 0 ; \tag{102}$$

the non-degeneracy of the GS implies that $e_s > 0$ for *all* $s \neq 0$. Thus we observe that the "poles" of the dynamical density-density correlation function are the energies of the N-electron excited states, as measured with respect to the N-electron GS energy ("neutral" excitations). We recall that for the "poles" of the GF we have, depending on whether $\varepsilon_s < \mu$ or $\varepsilon_s > \mu$, $\varepsilon_s = \mu_N - \bar{\varepsilon}_s$, with $\bar{\varepsilon}_s = E_{N-1,s} - E_{N-1,0}$, and $\varepsilon_s = \mu_{N+1} + \bar{\varepsilon}_s$, with $\bar{\varepsilon}_s = E_{N+1,s} - E_{N+1,0}$, respectively (see Subsec. 4.2). It is interesting to compare these two $\bar{\varepsilon}_s$'s with e_s in Eq. (102). From Eq. (100) it is obvious that $\chi(\varepsilon)$ can be written as $\chi(\varepsilon) = \overline{\chi}(\varepsilon) + \overline{\chi}(-\varepsilon)$, with $\overline{\chi}(\mathbf{r}, \mathbf{r}'; \varepsilon) := 2 \sum_s \varrho_s(\mathbf{r}) \varrho_s^*(\mathbf{r}')/(\varepsilon - e_s + i\eta)$, from which it follows that $\chi(-\varepsilon) \equiv \chi(\varepsilon)$.

Since the Hamiltonian of the system under consideration is time independent (after having set the possible $\varphi(\mathbf{r}t)$ in Subsec. 7.5 equal to zero), the two-point functions that occur in Eqs. (90)–(95) are functions of difference of their time arguments. Thus in the energy domain these functions depend only on one energy parameter. In this way Eq. (92) is directly transformed[70] into $W(\varepsilon) = v_c + v_c P(\varepsilon) W(\varepsilon)$. Similarly Eqs. (94) and (95) are transformed into $W(\varepsilon) = \epsilon^{-1}(\varepsilon) v_c$ and $\epsilon^{-1}(\varepsilon) = I + v_c \chi(\varepsilon)$, respectively. From these expressions, by *formal* algebraic manipulations, one obtains

$$\chi(\varepsilon) = P(\varepsilon)(I - v_c P(\varepsilon))^{-1} \equiv (P^{-1}(\varepsilon) - v_c)^{-1}\,, \tag{103}$$

or equivalently,

$$P(\varepsilon) = (I + \chi(\varepsilon) v_c)^{-1} \chi(\varepsilon) \equiv (\chi^{-1}(\varepsilon) + v_c)^{-1}\,. \tag{104}$$

From this result and $\chi(-\varepsilon) = \chi(\varepsilon)$ it follows that $P(-\varepsilon) = P(\varepsilon)$.

8.1. *Symmetries of χ and P*

From the many-body perturbation expansion for $P(\mathbf{r}, \mathbf{r}'; \varepsilon)$ in terms of either G_0 or G (in the latter case only the skeleton self-energy diagrams [see Footnote 26] are to be taken into account — see Fig. 10(a) and Fig. 11), and the symmetry property for these as presented in Eq. (25), it can be shown that (in absence of spin-polarisation and magnetic field [in the Coulomb gauge] — see Footnote 14 and Subsec. 4.4)

$$P(\mathbf{r}, \mathbf{r}'; \varepsilon) = P(\mathbf{r}', \mathbf{r}; \varepsilon)\,. \tag{105}$$

From this and Eq. (103) it follows that

$$\chi(\mathbf{r}, \mathbf{r}'; \varepsilon) = \chi(\mathbf{r}', \mathbf{r}; \varepsilon)\,. \tag{106}$$

There is one elegant way of demonstrating that under the above-mentioned conditions, the relation in Eq. (106) is indeed satisfied in the static limit (i.e. for $\varepsilon = 0$). This method is based on some elements of the DFT (Hohenberg and

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[70] We have to emphasise one important aspect involved here. The Fourier transform $F(\varepsilon)$ of $f(t)$ when back transformed, yields $f(t)$, excluding a set of measure zero: at point t_0, where $f(t)$ has a finite discontinuity, the back transformation yields $\frac{1}{2}\{f(t_0^+) + f(t_0^-)\}$ — recall that for $f(t)$ to have a Fourier transform, it is required that $f(t)$ possesses at most a *finite* number of *finite* discontinuities. This problem can be circumvented by *prescribing* a specific form for the contour of the energy integration in the complex energy plane for obtaining $f(t)$ from $F(\varepsilon)$ (better, from $\widetilde{F}(z)$), which of course requires analytic continuation of F into the z-plane (Subsec. 2.2). See, e.g., Fig. 4. This is important, since most of the correlation functions that we encounter in the many-body theory involve time-ordering operation, implying discontinuity in the t-domain. This explains the origin of Eqs. (28), (41) and (111).

Kohn 1964). Since in the present work we frequently encounter the DFT, it is useful to present this alternative demonstration. To this end we assume $w(\mathbf{r},\mathbf{r}') \equiv 0$, which is prerequisite[71] for having a DFT in terms of the GS electronic density $n(\mathbf{r})$. Owing to the one-to-one relationship between the GS density $n(\mathbf{r})$ and the local external potential $v(\mathbf{r})$, the usual expression for the GS total energy functional within the DFT (Hohenberg and Kohn 1964),

$$E_v[n] = \int d^3r\, v(\mathbf{r}) n(\mathbf{r}) + F[n]\,, \tag{107}$$

with $F[n]$ a *universal* functional of the density (i.e., $F[n]$ does not explicitly depend on the external potential v), can be viewed as a Legendre transform (Lieb 1983) between $n(\mathbf{r})$ and $v(\mathbf{r})$. Let therefore $E[v]$ denote $E_v[n]$ when the GS total energy is viewed as a functional of v. From Eq. (107) we have

$$n(\mathbf{r}) = \frac{\delta E[v]}{\delta v(\mathbf{r})}\,. \tag{108}$$

Now since $\chi(\mathbf{r},\mathbf{r}';\varepsilon = 0) := \delta n(\mathbf{r})/\delta v(\mathbf{r}')$, from Eq. (108) we obtain

$$\chi(\mathbf{r},\mathbf{r}';\varepsilon = 0) = \frac{\delta^2 E[v]}{\delta v(\mathbf{r}) \delta v(\mathbf{r}')}\,. \tag{109}$$

Since for a twice-differentiable functional the order of carrying out the (functional) differentiation is immaterial, Eq. (109) demonstrates the symmetry relation in Eq. (106) concerning $\varepsilon = 0$. For $\varepsilon \neq 0$, one can similarly proceed by making use of a Legendre transform that is analogous to that in Eq. (107) within the framework of the time-dependent DFT. We shall encounter this theory in Subsubsec. 8.6.2.

8.2. *Analytic continuation of $\chi(\varepsilon)$, $\widetilde{\chi}(z)$; analyticity and its consequences*

Let us define[72]

$$\widetilde{\chi}(\mathbf{r},\mathbf{r}';z) := 4 \sum_s e_s \frac{\varrho_s(\mathbf{r})\varrho_s^*(\mathbf{r}')}{z^2 - e_s^2}\,. \tag{110}$$

It is easily verified that $\chi(\varepsilon)$ on the RHS of

$$\lim_{\eta \downarrow 0} \widetilde{\chi}(\varepsilon \pm i\eta) \equiv \chi(\varepsilon)\,, \quad \text{when } \varepsilon \gtrless 0 \tag{111}$$

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[71] Only a *local* external potential can be in a one-to-one correspondence with $n(\mathbf{r})$.

[72] Similar to ε_s in Subsec. 4.4, here for every s there exists an $\overline{s}$ for which holds $e_{\overline{s}} = e_s$ — Kramers' degeneracy (see specifically Footnote 21).

coincides with $\chi(\varepsilon)$ in Eq. (100). Thus $\widetilde{\chi}(z)$ is the analytic continuation of $\chi(\varepsilon)$ into the the physical RS of the complex z-plane (see Subsec. 2.2). From Eq. (110) it is obvious that $\widetilde{\chi}(-z) = \widetilde{\chi}(z)$, i.e. similar to $\chi(\varepsilon)$, $\widetilde{\chi}(z)$ is an *even* function of its argument.

Since $\widetilde{\chi}(z)$ is analytic everywhere on the complex z-plane, with the possible exception of the real axis, and since, following Eq. (110), $\widetilde{\chi}(z)$ decreases like $1/z^2$ for $|z| \to \infty$, there exists an identical expression for $\widetilde{\chi}(z)$ as for $\widetilde{\Sigma}_r(z)$ that we have presented in Eq. (45). Let therefore (see Footnote 27)

$$\widetilde{\chi}'(z) := \frac{1}{2}\{\widetilde{\chi}(z) + \widetilde{\chi}^{\dagger}(z)\}\,, \quad \widetilde{\chi}''(z) := \frac{1}{2i}\{\widetilde{\chi}(z) - \widetilde{\chi}^{\dagger}(z)\} \tag{112}$$

be the "real" and "imaginary" parts of $\widetilde{\chi}(z)$. The counterpart of Eq. (45) for $\widetilde{\chi}(z)$ can be written as the following pair of Kramers–Kronig-type of expressions (*c.f.* Eq. (48))

$$\begin{aligned}\widetilde{\chi}'(\varepsilon \pm i\eta) &= \pm\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\varepsilon' \frac{\widetilde{\chi}''(\varepsilon' \pm i\eta)}{\varepsilon' - \varepsilon}\,,\\ \widetilde{\chi}''(\varepsilon \pm i\eta) &= \mp\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\varepsilon' \frac{\widetilde{\chi}'(\varepsilon' \pm i\eta)}{\varepsilon' - \varepsilon}\,.\end{aligned} \tag{113}$$

This pair is verified correctly to satisfy

$$\widetilde{\chi}'(z^*) = \widetilde{\chi}'(z)\,, \quad \widetilde{\chi}''(z^*) = -\widetilde{\chi}''(z)\,; \tag{114}$$

these expressions are direct consequences of $\widetilde{\chi}^{\dagger}(z) \equiv \widetilde{\chi}(z^*)$ — this relation follows from Eqs. (106) and (110). The expressions in Eq. (113) are not exclusively in terms of the *physical* density-density correlation function. For obtaining a pair of expressions entirely in terms of the latter, we make use of Eq. (114). After some algebra, from Eq. (113) the desired Kramers-Kronig-type of expressions for the *physical* χ (see Eq. (100)) are shown to be

$$\begin{aligned}\chi'(\varepsilon) &= -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\varepsilon' \frac{\mathrm{sgn}(-\varepsilon')\chi''(\varepsilon')}{\varepsilon' - \varepsilon}\,,\\ \chi''(\varepsilon) &= \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\varepsilon' \frac{\mathrm{sgn}(-\varepsilon)\chi'(\varepsilon')}{\varepsilon' - \varepsilon}\,.\end{aligned} \tag{115}$$

These expressions are, except for a μ whose place has been taken by zero, formally identical to those in Eq. (50).

8.3. Large-$|\varepsilon|$ limits

From Eq. (100) it directly follows that

$$\begin{aligned}\chi(\mathbf{r},\mathbf{r}';\varepsilon) &= \frac{4}{\varepsilon^2}\sum_s e_s \varrho_s(\mathbf{r})\varrho_s^*(\mathbf{r}') + \mathcal{O}(\varepsilon^{-4})\\ &\equiv \frac{2}{\varepsilon^2}\sum_s e_s\left\{\varrho_s(\mathbf{r})\varrho_s^*(\mathbf{r}') + \varrho_s(\mathbf{r}')\varrho_s^*(\mathbf{r})\right\} + \mathcal{O}(\varepsilon^{-4}), \quad \text{for } |\varepsilon| \to \infty .\end{aligned} \tag{116}$$

In the second expression we have made the symmetry property in Eq. (106) explicit. The even powers of $1/\varepsilon$ in this expression reflect the fact that $\chi(\varepsilon)$ is an *even* function of ε (see Eq. (100)). From Eq. (116) one readily observes that for sufficiently large $|\varepsilon|$, $\chi(\varepsilon)$ is positive semi-definite. On the other hand it can readily be verified from Eq. (100) that for sufficiently small $|\varepsilon|$, $\chi(\varepsilon)$ is negative semi-definite (were it not because of $\varrho_{s=0}(\mathbf{r}) \equiv 0$, or $e_{s=0} = 0$, $\chi(\varepsilon)$ in the latter two cases were, respectively, positive definite and negative definite). Thus in changing $|\varepsilon|$ from 0 to ∞, except for a zero eigenvalue, *all* eigenvalues of $\chi(\varepsilon)$ shift from below to above zero. This implies that for $|\varepsilon|$ above certain value, for which $\chi(\varepsilon)$ is no longer negative semi-definite, the system does *not* behave quasi-statically (see Subsucsec 8.6.2).

From Eq. (104) we deduce

$$P(\mathbf{r},\mathbf{r}';\varepsilon) = \chi(\mathbf{r},\mathbf{r}';\varepsilon) + \mathcal{O}(\varepsilon^{-4}), \quad \text{for } |\varepsilon| \to \infty . \tag{117}$$

From the second expression in Eq. (116), making use of Eq. (101) and the fact that $E_{N,s}|\Psi_{N,s}\rangle = \widehat{H}|\Psi_{N,s}\rangle$, we readily arrive at

$$\lim_{|\varepsilon|\to\infty} \varepsilon^2\chi(\mathbf{r},\mathbf{r}';\varepsilon) =: \chi_{\infty_2}(\mathbf{r},\mathbf{r}') = -2\langle\Psi_{N,0}|\left[\left[\widehat{H},\widehat{n}(\mathbf{r})\right]_-,\widehat{n}(\mathbf{r}')\right]_-|\Psi_{N,0}\rangle , \tag{118}$$

where we have, in addition, made use of the completeness relation for the eigenstates of $\widehat{H}$. In Eq. (118) we have introduced the number-density operator

$$\widehat{n}(\mathbf{r}) := \widehat{\psi}^\dagger(\mathbf{r})\widehat{\psi}(\mathbf{r}). \tag{119}$$

On the other hand, the total electronic density in the GS is defined according to

$$n(\mathbf{r}) := 2\langle\Psi_{N,0}|\widehat{n}(\mathbf{r})|\Psi_{N,0}\rangle , \tag{120}$$

where the factor 2 on the RHS accounts for the trace over the spin states of an electron. Note that since $\widehat{n}(\mathbf{r})$ and $\widehat{n}(\mathbf{r}')$ commute, the RHS of Eq. (118) is indeed symmetric with respect to transposition of $\mathbf{r}$ and $\mathbf{r}'$. Through some straightforward algebra, making use of the anti-commutation relations for the field operators, one obtains[73]

$$\begin{aligned}
[[\widehat{T},\widehat{n}(\mathbf{r})]_-,\widehat{n}(\mathbf{r}')]_- &= \frac{\hbar^2}{m_e}\boldsymbol{\nabla}\cdot[\widehat{n}(\mathbf{r})\boldsymbol{\nabla}\delta(\mathbf{r}-\mathbf{r}')]\,,\\
[[\widehat{U}_v,\widehat{n}(\mathbf{r})]_-,\widehat{n}(\mathbf{r}')]_- &= \widehat{0}\,,\\
[[\widehat{U}_w,\widehat{n}(\mathbf{r})]_-,\widehat{n}(\mathbf{r}')]_- &= \delta(\mathbf{r}-\mathbf{r}')\int d^3r''w(\mathbf{r},\mathbf{r}'')\{\widehat{\psi}^\dagger(\mathbf{r}'')\widehat{\psi}(\mathbf{r})+\widehat{\psi}^\dagger(\mathbf{r})\widehat{\psi}(\mathbf{r}'')\}\\
&\quad - w(\mathbf{r},\mathbf{r}')\{\widehat{\psi}^\dagger(\mathbf{r})\widehat{\psi}(\mathbf{r}')+\widehat{\psi}^\dagger(\mathbf{r}')\widehat{\psi}(\mathbf{r})\}\,,\\
[[\widehat{V},\widehat{n}(\mathbf{r})]_-,\widehat{n}(\mathbf{r}')]_- &= \widehat{0}\,. \qquad (121)
\end{aligned}$$

Thus Eq. (118) can be written as

$$\begin{aligned}
\lim_{|\varepsilon|\to\infty}\varepsilon^2\chi(\mathbf{r},\mathbf{r}';\varepsilon) =: \chi_{\infty_2}(\mathbf{r},\mathbf{r}') &= \frac{-\hbar^2}{m_e}\boldsymbol{\nabla}\cdot[n(\mathbf{r})\boldsymbol{\nabla}\delta(\mathbf{r}-\mathbf{r}')] - 2\delta(\mathbf{r}-\mathbf{r}')\\
&\quad\times\int d^3r''w(\mathbf{r},\mathbf{r}'')\rho(\mathbf{r}'',\mathbf{r}) + 2w(\mathbf{r},\mathbf{r}')\rho(\mathbf{r},\mathbf{r}')\,, \qquad (122)
\end{aligned}$$

where the reduced single-particle density matrix $\rho(\mathbf{r},\mathbf{r}')$ has already been defined in Eq. (16). In arriving at the above result we have explicitly made use of the symmetry relation in Eq. (26).

From Eq. (117) it follows that

$$\lim_{|\varepsilon|\to\infty}\varepsilon^2\{\chi(\varepsilon)-P(\varepsilon)\}=0 \iff \chi_{\infty_2}\equiv P_{\infty_2}\,, \qquad (123)$$

so that the RHSs of Eqs. (118) and (122) also apply to $P_{\infty_2}(\mathbf{r},\mathbf{r}')$.

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[73] As a hint, we mention that the double commutation expressions in Eq. (121), in particular the first one [which, because of the ∇^2 in $\widehat{T}$, may be experienced as un-inviting], are easiest obtained through employing the representations of the creation and annihilation field operators in terms on a complete set of one-particle wavefunctions, namely: $\widehat{\psi}^\dagger(\mathbf{r})=\sum_i\psi_i^*(\mathbf{r})\widehat{c}_i^\dagger$ and $\widehat{\psi}(\mathbf{r})=\sum_i\psi_i(\mathbf{r})\widehat{c}_i$, where the operators $\widehat{c}_i^\dagger$, $\widehat{c}_i$ satisfy the fermionic anti-commutation relations $[\widehat{c}_i^\dagger,\widehat{c}_j]_+=\delta_{i,j}$, $[\widehat{c}_i^\dagger,\widehat{c}_j^\dagger]_+=0$ and $[\widehat{c}_i,\widehat{c}_j]_+=0$.

8.4. *Perturbation expansion for the polarisation function* P; $P^{\{0\}}$ *and* $P^{\{1\}}$

Through application of the many-body perturbation theory (or through a systematic formal solution of Eqs. (90)–(93)) one observes that P can be written as $P = P_0 + P_1$, where P_0 does not *explicitly* depend on the electron-electron interaction function v_c. Here P_0 and P_1 are functionals of G, the *exact* GF. Employing the notation introduced in Subsec. 7.6, we can thus write $P^{\{1\}}[G] = P_0^{\{1\}}[G] + P_1^{\{1\}}[G]$ where $P_0(1,2;[G]) = (-2i/\hbar)G(1,2^+)G(2,1)$. Through further expanding G in terms of G_0, the GF pertaining to some appropriate non-interacting Hamiltonian, one can write P as a functional of G_0, $P^{\{0\}}[G_0] = P_0^{\{0\}}[G_0] + P_1^{\{0\}}[G_0]$. We have $P_0^{\{0\}}[F] \equiv P_0^{\{1\}}[F]$, so that superscripts $\{0\}$ and $\{1\}$ attached to P_0 may be suppressed.

The Feynman diagram representing P_0 has the shape of a loop or "bubble" (see Fig. 12(a)), so that P_0 is sometimes referred to as the "bubble approximation" for P; it is also referred to as the random-phase approximation, RPA, for P (Pines and Bohm 1952, Bohm and Pines 1953, Pines and Nozières 1966, pp. 279–341). Traditionally, the RPA refers to $P_0[G_0]$ with G_0 the GF of the self-consistent one-electron Hartree Hamiltonian. For the uniform-electron system, the Hartree potential (which is divergent) exactly cancels the (equally divergent) potential corresponding to the interaction of electrons with the

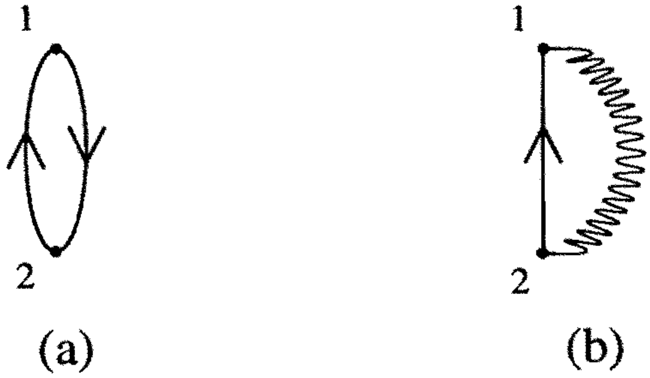

Fig. 12. (a) Diagrammatic representation of the Random-Phase approximation (RPA) for the polarisation function P, and (b) of the dynamically-screened exchange, or GW, approximation for the self-energy operator. The directed solid line from j to i stands for the single-particle Green function $G(i,j)$ and the wavy line for W (whence the "GW" approximation). If the solid line is taken to represent G_0, the single-particle Green function pertaining to some "non-interacting" Hamiltonian, then diagram (a) represents the exact density-density correlation function χ_0 of the corresponding "non-interacting" system. In the main text, by χ_0 we denote the density-density response function pertaining to the "non-interacting" Kohn-Sham Hamiltonian.

positively-charged background. Consequeutly, for the uniform-electron system, G_0 within the self-consistent Hartree approximation is (up to a global gauge transformation) identical with that of the non-interacting electrons. Therefore, for this system the RPA for P coincides with the Lindhard (1954) polarisation function (Ashcroft and Mermin 1981, pp. 343 and 344). In the following Sections we shall denote $P_0[G_0]$ by χ_0 when G_0 coincides with the GF of the 'non-interacting' KS Hamiltonian (see Eq. (135) below). For a system with a uniform GS charge density, the effective potential in the associated KS Hamiltonian is a constant, so that (up to a trivial phase factor) G_{KS} is identical with the G_0 pertaining to the uniform system of non-interacting electrons. Therefore the χ_0 pertaining to a uniform KS system is also identical with the Lindhard polarisation function.

8.5. *Random-Phase Approximation, RPA, and large* $|\varepsilon|$

For the time being we shall specifically deal with $P_0[G]$. From $P_0(1,2) = (-2i/\hbar)G(1,2^+)G(2,1)$ for $P_0(\mathbf{r},\mathbf{r}';\varepsilon)$ we have:

$$P_0(\mathbf{r},\mathbf{r};\varepsilon) = \frac{-2i}{\hbar}\int_{-\infty}^{\infty}\frac{d\varepsilon'}{2\pi\hbar}G(\mathbf{r},\mathbf{r}';\varepsilon')G(\mathbf{r}',\mathbf{r};\varepsilon'-\varepsilon)e^{i\eta'\varepsilon'/\hbar}, \quad (\eta'\downarrow 0), \quad (124)$$

where the exponential fnnction (which is due to 2^+ in $G(1,2^+)$), can be set to unity. This is because "+" in 2^+ is the remnant of an *ad hoc* measure taken for avoiding the time-ordering ambiguities that arise in consequence of the instantaneous nature of the bare two-particle (Coulomb) interaction. Here changing 2^+ into 2 does *not* lead to any ambiguity. This is closely related to the fact that $G(\varepsilon')G(\varepsilon'-\varepsilon) \sim \hbar^2 I/\varepsilon'^2$ for $|\varepsilon'| \to \infty$, so that $P_0(\mathbf{r}t,\mathbf{r}'t')$, which is a function of $\tau := t - t'$, is *continuous* at $\tau = 0$ (see Appendix B). Employing the Lehmann representation for $G(\varepsilon)$ in Eq. (11) and making use of the Cauchy residue theorem (Titchmarsh 1939, p. 102) it can readily be shown that similar to $\chi(\varepsilon)$,

$$P_0(\mathbf{r},\mathbf{r}';\varepsilon) = \overline{P}_0(\mathbf{r},\mathbf{r}';\varepsilon) + \overline{P}_0(\mathbf{r},\mathbf{r}';-\varepsilon), \quad (125)$$

where

$$\overline{P}_0(\mathbf{r},\mathbf{r}';\varepsilon) := 2\sum_s^{>}\sum_{s'}^{<}\frac{f_s(\mathbf{r})f_s^*(\mathbf{r}')f_{s'}(\mathbf{r}')f_{s'}^*(\mathbf{r})}{\varepsilon+\varepsilon_{s'}-\varepsilon_s+i\eta}, \quad (\eta\downarrow 0). \quad (126)$$

Here we have introduced the short-hand notations $\sum_s^{>}(\ldots)$ and $\sum_{s'}^{<}(\ldots)$ for $\sum_s \theta(\varepsilon_s-\mu)(\ldots)$ and $\sum_{s'}\theta(\mu-\varepsilon_{s'})(\ldots)$, respectively.

Let us now investigate the asymptotic behaviour of $P_0(\varepsilon)$ for $|\varepsilon| \to \infty$. Through some simple algebra (in particular by making explicite use of the symmetry relation $P(\mathbf{r}, \mathbf{r}'; \varepsilon) = P(\mathbf{r}', \mathbf{r}; \varepsilon)$ — Eq. (105)), it follows that

$$\lim_{|\varepsilon| \to \infty} \varepsilon^2 P_0(\mathbf{r}, \mathbf{r}'; \varepsilon) = 4 \sum_{s}^{>} \sum_{s'}^{<} (\varepsilon_s - \varepsilon_{s'}) f_s(\mathbf{r}) f_s^*(\mathbf{r}') f_{s'}(\mathbf{r}') f_{s'}^*(\mathbf{r}) \,. \tag{127}$$

Using the definitions for the Lehmann amplitudes and energies (Eqs. (12) and (13)) we readily obtain (see Eqs. (118), (123) above and Eq. (152) below)[74]

$$\begin{aligned} \lim_{|\varepsilon| \to \infty} \varepsilon^2 P_0(\mathbf{r}, \mathbf{r}'; \varepsilon) &=: P_{0;\infty_2}(\mathbf{r}, \mathbf{r}') \\ &= -2\langle \Psi_{N,0} | [[\widehat{H}, \widehat{n}(\mathbf{r})]_-, \widehat{n}(\mathbf{r}')]_- | \Psi_{N,0} \rangle + R(\mathbf{r}, \mathbf{r}') \\ &\equiv P_{\infty_2}(\mathbf{r}, \mathbf{r}') + R(\mathbf{r}, \mathbf{r}') \equiv \chi_{\infty_2}(\mathbf{r}, \mathbf{r}') + R(\mathbf{r}, \mathbf{r}') \,, \end{aligned} \tag{128}$$

where[75]

$$\begin{aligned} R(\mathbf{r}, \mathbf{r}') &:= v_c(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}, \mathbf{r}') \\ &\quad - \left\{ 4 \int d^3 r'' v_c(\mathbf{r} - \mathbf{r}'') \left[2 \sum_s \varrho_s(\mathbf{r}) \varrho_s^*(\mathbf{r}'') \right] \right\} \delta(\mathbf{r} - \mathbf{r}') \,. \end{aligned} \tag{129}$$

The *explicit* dependence of $R(\mathbf{r}, \mathbf{r}')$ on v_c, as exposed by the RHS of Eq. (129), is due to our evaluation of P_0 in terms of the *exact* GF. This implies that the pertinent expression for $P_{0;\infty_2}[G_0]$ functionally differs from that in Eq. (128) by the absence of a corresponding R in it, even for cases where G_0 would *implicitly* depend on v_c (such as is the case for, e.g., the G_0 pertaining to the Hartree one-particle Hamiltonian which depends *implicitly* on v_c via the Hartree potential). As a consequence of this and in view of Eqs. (122)[76] and (128), we

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[74] I am indebted to Professor Lars Hedin for pointing out an omission in the original version of this expression.

[75] In arriving at Eq. (128) we have made use of $\int d^3 r'' v_c(\mathbf{r} - \mathbf{r}'') \langle \Psi_{N,0} | \widehat{\psi}^\dagger(\mathbf{r}) \widehat{\psi}^\dagger(\mathbf{r}'') \widehat{\psi} \cdot (\mathbf{r}'') \widehat{\psi}(\mathbf{r}) | \Psi_{N,0} \rangle = \int d^3 r'' v_c(\mathbf{r} - \mathbf{r}'') \langle \Psi_{N,0} | \widehat{n}(\mathbf{r}) \widehat{n}(\mathbf{r}'') | \Psi_{N,0} \rangle = \frac{1}{2} n(\mathbf{r}) v_H(\mathbf{r}; [n]) + \int d^3 r'' v_c(\mathbf{r} - \mathbf{r}'') [2 \sum_s \varrho_s(\mathbf{r}) \varrho_s^*(\mathbf{r}'')]$. We have multiplied the RHS of this expression by 2 in order to account for the internal spin degree of freedom. Further, the second expression follows from the first after application of the process of normal ordering.

[76] Note the important fact that the RHS of Eq. (122) has no *explicit* dependence on the electron-electron interaction function v_c.

arrive at a most remarkable result, namely that provided G_0 yields the exact ground-state $n(\mathbf{r})$ and $\rho(\mathbf{r},\mathbf{r}')$ [see further on], $P_{0;\infty_2}[G_0]$ exactly reproduces the leading-order asymptotic term of $\chi(\varepsilon)$ for $|\varepsilon| \to \infty$; from Eq. (123) it follows that in such an event, $P_{0;\infty_2}[G_0]$ also exactly reproduces the leading-order asymptotic term of $P(\varepsilon)$ for $|\varepsilon| \to \infty$. For cases where $w(\mathbf{r},\mathbf{r}') \equiv 0$, a G_0 that yields the exact $n(\mathbf{r})$ will suffice. Such a G_0 is by definition the GF of the non-interacting KS system, i.e. G_{KS},[77] that features within the context of the ground-state DFT (Hohenberg and Kohn 1964, Kohn and Sham 1965) — Subsecs. 8.1 and 8.6. For construction of a G_0 that would yield the exact $\rho(\mathbf{r},\mathbf{r}')$, one would have to resort to the DFT for non-local external potentials, first introduced by Gilbert (1975); in Subsec. 9.7 we shall briefly encounter this formalism. Within the framework of the latter DFT, it is however necessary to deal with an ensemble of eigenstates of the pertinent "non-interacting" KS Hamiltonian.[78]

The above considerations lead us to a further important result, namely that when calculation of $P(\varepsilon)$ is restricted to the zeroth-order term $P_0(\varepsilon)$, it is preferable, at least when $w(\mathbf{r},\mathbf{r}') \equiv 0$, to evaluate $P_0(\varepsilon)$ in terms of G_{KS} rather than G (assuming that G were known): When $w(\mathbf{r},\mathbf{r}') \equiv 0$, $P_{0;\infty_2}[G_{KS}] \equiv P_{\infty_2}$ but $P_{0;\infty_2}[G] \not\equiv P_{\infty_2}$. We recall that $\chi_0{:=}P_0[G_{KS}]$, so that, following Eq. (123) above, we equivalently have: $\chi_{0;\infty_2} \equiv \chi_{\infty_2}$, that is, for large $|\varepsilon|$, the leading-order asymptotic contribution of the density-density response function of the "non-interacting" KS system is identical with that of the interacting system (Farid 1999b).

8.6. *On aspects of the density-functional theory*

In view of the importance of G_{KS}, the GF of the KS Hamiltonian (see particularly Subsec. 8.5), below we briefly present two DFTs. In both cases we have to make the assumption that $w(\mathbf{r},\mathbf{r}') \equiv 0$. In Subsec. 9.7 we touch upon the DFT appropriate to the cases where $w(\mathbf{r},\mathbf{r}') \not\equiv 0$.

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[77] Recall our convention in Subsec. 8.4, that for G_0 coinciding with G_{KS}, we denote $P_0[G_0]$ by χ_0. See Subsec. 8.6.1.

[78] We have to point out that in this context "KS Hamiltonian" is not an appropriate designation. This is owing to the fact that within Gilbert's framework, the pertinent Schrödinger equation for the "natural orbitals" *directly* follows from the Euler-Lagrange equation for the total-energy functional, without reliance on the intermediate step of introducing $T_s[n]$, the kinetic-energy functional pertaining to the KS system of ficticious non-interacting particles; in Gilbert's formalism one encounters the kinetic energy of the *interacting* system, which is an explicit functional of ρ.

8.6.1. *The ground-state DFT*

The *ground-state* DFT yields the exact $\chi(\varepsilon = 0)$ via a second-order functional derivative of the GS total energy viewed as a functional of the local external potential v (see Eq. (109) above). Using the fact that the *static* density-density correlation function of the KS system, χ_0, is defined through

$$\chi_0(\mathbf{r}, \mathbf{r}') := \frac{\delta n(\mathbf{r})}{\delta v_{\text{eff}}(\mathbf{r}'; [n])}, \tag{130}$$

in contrast to the static χ which is defined by

$$\chi(\mathbf{r}, \mathbf{r}') := \frac{\delta n(\mathbf{r})}{\delta v(\mathbf{r}')} \tag{131}$$

(in the static limit, the variation of the *actual* static external potential v is equivalent with that of the auxiliary potential φ as introduced in Subsec. 7.5), where (Kohn and Sham 1965)

$$v_{\text{eff}}(\mathbf{r}; [n]) := v(\mathbf{r}) + v_H(\mathbf{r}; [n]) + v_{xc}(\mathbf{r}; [n]). \tag{132}$$

Here $v_H(\mathbf{r}; [n])$ is the Hartree potential defined in Eq. (24) and $v_{xc}(\mathbf{r}; [n]) := \delta E_{xc}[n]/\delta n(\mathbf{r})$ stands for the exchange-correlation potential, with $E_{xc}[n]$ the exchange-correlation energy functional (see Subsec. 9.7). By the chain rule of functional differentiation it is easily shown that the following Dyson-type equation holds for the *static* χ and χ_0:

$$\chi = \chi_0 + \chi_0 C \chi. \tag{133}$$

Here the two-point function C is defined as follows

$$C(\mathbf{r}, \mathbf{r}'; [n]) := v_c(\mathbf{r} - \mathbf{r}') + K_{xc}(\mathbf{r}, \mathbf{r}'; [n]), \text{ with } K_{xc}(\mathbf{r}, \mathbf{r}'; [n]) := \frac{\delta v_{xc}(\mathbf{r}; [n])}{\delta n(\mathbf{r}')}. \tag{134}$$

Owing to the fact that $v_{xc}(\mathbf{r}; [n]) := \delta E_{xc}[n]/\delta n(\mathbf{r})$, we have $C(\mathbf{r}, \mathbf{r}') = C(\mathbf{r}', \mathbf{r})$.

From Eq. (130) and the fact that $n(\mathbf{r}) = -2iG(\mathbf{r}t, \mathbf{r}t^+) \equiv -2iG_{KS}(\mathbf{r}t, \mathbf{r}t^+)$, it immediately follows that indeed $\chi_0(\mathbf{r}, \mathbf{r}') \equiv P_0(\mathbf{r}, \mathbf{r}'; \varepsilon = 0; [G_{KS}])$ — see Eq. (135) below. As a consequence, the *static* χ_0 is easily generalised to the *dynamic* χ_0: This function, $\chi_0(\mathbf{r},\mathbf{r}';\varepsilon)$, is obtained from Eqs. (125), (126) by means of replacing $f_s(\mathbf{r})$ by $\psi_i(\mathbf{r})$ and ε_s by ε_i, where $\psi_i(\mathbf{r})$ and ε_i are the one-particle eigenfunctions and eigenvalues of the self-consistent KS Hamiltonian:

$$\left[\frac{-\hbar^2}{2m_e}\nabla^2 + v_{\text{eff}}(\mathbf{r};[n])\right]\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})\,,$$

$$n(\mathbf{r}) = 2\sum_i \theta(\mu-\varepsilon_i)\psi_i(\mathbf{r})\psi_i^*(\mathbf{r})\,. \qquad (135)$$

Here μ is determined by the requirement $\sum_i \theta(\mu-\varepsilon_i) = N$. By retaining C in Eq. (133) as defined in Eq. (134), but replacing the static χ_0 by the *dynamic* $\chi_0(\varepsilon)$ we have the following approximate $\chi(\varepsilon)$:

$$\chi(0) \to \chi_{\text{gs}}(\varepsilon) := (I-\chi_0(\varepsilon)C)^{-1}\chi_0(\varepsilon) \equiv \chi_0(\varepsilon)(I-C\chi_0(\varepsilon))^{-1}\,, \qquad (136)$$

which yields the *exact* $\chi(0)$ as $|\varepsilon| \to 0$ ("gs" denotes "ground state"). Moreover, owing to Eq. (128) and the above-discussed property (Subsec. 8.5 — see text following Eq. (129)) concerning $P_0(\varepsilon)$ as evaluated in terms of G_{KS} (which coincides with $\chi_0(\varepsilon)$), we observe that $\chi_{\text{gs}}(\varepsilon)$ yields also the leading-order term pertaining to $\chi(\varepsilon)$ as $|\varepsilon| \to \infty$. It follows that the DFT is not only an *exact* theory concerning $|\varepsilon| \to 0$, *but*, as far as the charge response of the system is concerned, also one concerning $1/|\varepsilon| \to 0$. It is interesting to note that since $\chi(\varepsilon)$ and $\chi_0(\varepsilon)$ are *even* functions of ε, the deviation of $\chi_{\text{gs}}(\varepsilon)$ from the exact $\chi(\varepsilon)$ concerns terms of order ε^2 and $1/\varepsilon^4$ for small and large values of $|\varepsilon|$, respectively.

The above observations are in support of our statement in Subsubsec. 7.4.1 that many-body PTs based on the pertinent KS "unperturbed" Hamiltonians are unconditionally valid (assuming of course that certain GS densities, such as $n(\mathbf{r})$, are pure-state non-interacting v-representable).

From Fig. 10(a) and Fig. 11 it is obvious that the difference between P and P_0 (i.e. P_1 — see Subsec. 8.4) originates from the difference between the vertex function $\Gamma(1,2;3)$ and $\delta(1,2)\delta(1,3)$. The first attempt to incorporating this difference is due to Hubbard (1958). It turns out that the approximate approach introduced by Hubbard (1958) can be put on a firm theoretical basis within the framework of the (ground-state) DFT: In the static limit, Hubbard's local-field function, the so-called G-function, can be shown to be related to K_{xc}

(see Eq. (134)) as follows:[79]

$$K_{xc} = -v_c \mathrm{G}\,. \tag{137}$$

We shall consider the G-function in Subsubsec. 8.6.3.

8.6.2. *The time-dependent DFT*

In Subsubsec. 8.6.1 we have shown that $\chi_{\mathrm{gs}}(\varepsilon)$ in principle only in two (asymptotic) limits yields the correct $\chi(\varepsilon)$: $|\varepsilon| \to 0$ and $|\varepsilon| \to \infty$. That the static limit is reproduced correctly is natural, since $\chi(\varepsilon = 0)$ *is* a GS property. Within the framework of the time-dependent DFT (Runge and Gross 1984), K_{xc} and therefore C, in Eq. (134), become time-dependent operators and one naturally has an extension of $\chi_{\mathrm{gs}}(\varepsilon)$ in Eq. (136), formally effected through replacing C by $C(\varepsilon)$, which we denote by $\chi_{\mathrm{td}}(\varepsilon)$; here "td" stands for "time dependent". We have

$$\chi_{\mathrm{td}}(\varepsilon) := (I - \chi_0(\varepsilon) C(\varepsilon))^{-1} \chi_0(\varepsilon) \equiv \chi_0(\varepsilon)(I - C(\varepsilon)\chi_0(\varepsilon))^{-1}\,. \tag{138}$$

Barring fundamental problems (see further on) (Gross and Kohn 1985, Gross 1990) $\chi_{\mathrm{td}}(\varepsilon) \equiv \chi(\varepsilon)$ holds. We point out that the time-dependent DFT is valid for only a *restricted* set of time-dependent external potentials, so that the equality of the two response functions is not absolute but only relative with respect to this set of time-dependent external potentials; this restriction is associated with the possibility of the non-interacting non-v-representability [see Footnote 7] of the time-dependent electron density of an interacting system — for details see, e.g., work by Gross (1990). Stated differently, whether $\chi_{\mathrm{td}}(\varepsilon) \equiv \chi(\varepsilon)$ or not, crucially depends on whether $\chi_0^{-1}(\varepsilon) - \chi^{-1}(\varepsilon) =: C(\varepsilon)$ exists or not (Mearns and Kohn 1987). In the static case, addressed by the GS DFT, one is confronted with the same problem, however here singularity of $\chi(\varepsilon = 0)$ stands on a par with the instability of the GS of the system, which can be ruled out by the assumption of non-degeneracy of this state.[80] According to Mearns and Kohn (1987) (see also Gross, Mearns and Oliveira (1988) and

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[79] Hubbard's original G-function has the simple form $\mathrm{G}_H(k) = k^2/(2[k^2 + k_F^2])$. Hubbard's modified G-function (as reported in Kleinman (1967)) has the form: $\mathrm{G}_H^{\mathrm{mod}}(k) = k^2/(2[k^2 + k_F^2 + k_s^2])$, where k_s denotes the inverse of some screening length. For $k \to \infty$, both of these functions approach 1/2.

[80] For closed systems, both $\chi(\varepsilon = 0)$ and $\chi_0(\varepsilon = 0)$ have a zero eigenvalue, corresponding to a spatially constant eigenfunction. This follows from the observation that a constant potential cannot change the total number of electrons in these systems. Thus by excluding this

Ng and Singwi (1987)), $C(\varepsilon)$ exists *only* for $|\varepsilon| < \varepsilon_{\min}$, where $\varepsilon_{\min}$ denotes the lowest neutral-excitation energy of the system. Thus *in general* $\chi_{\mathrm{td}}(\varepsilon) \not\equiv \chi(\varepsilon)$.

8.6.3. *The local-field function* G

In the past, many attempts have been devoted to evaluating $\mathsf{G}(k)$ and $\mathsf{G}(k;\varepsilon)$ — which is associated with $C(\varepsilon)$ in Subsubsec. 8.6.2 —, the static and dynamic local-field-correction functions, respectively, pertaining to the uniform-electron system. For a review see the work by Farid, Heine, Engel and Robertson (1993). Concerning the behaviour of $\mathsf{G}(k;0) \equiv \mathsf{G}(k)$, for small values of k all the available models correctly[81] yield $\mathsf{G}(k;0) \propto k^2$. This is in particular the case within the framework of the LDA, where K_{xc} is a negative constant, i.e. independent of k, so that from Eq. (137) it follows that $\mathsf{G}_{LDA}(k) \propto k^2$ for *all* values of k. This behaviour, that $\mathsf{G}_{LDA}(k) > 1$ for large values of k (i.e., for $k \gg k_F$), had for long been considered as "completely wrong" (Taylor 1978). This judgement has its origin in two expressions — relating the behaviour of $\mathsf{G}(k)$ at large k with that of the electronic pair-correlation function for the interacting system, $g(\varrho)$, at small distance $\varrho := \|\mathbf{r}-\mathbf{r}'\|$ (see Subsec. 8.8) — due to Shaw (1970) and Niklasson (1974). The Shaw relation reads $\mathsf{G}(k \to \infty) = 1 - g(\varrho \to 0)$, and that by Niklasson $\mathsf{G}(k \to \infty) = 2[1 - g(\varrho \to 0)]/3$. Both of these imply that, since $g(\varrho) \in (0,1)$, $0 < \mathsf{G}(k \to \infty) < 1$. Holas (1987, 1991) has shown that these two relations are consequences of *partial* incorporation of correlation effects in the expressions for χ_0 as employed by Shaw and Niklasson — in other words, while often not fully realised (as evidenced by a wealth of incorrect results in the literature), the G-function in different works describe *different* correlation effects.[82] Thus Holas has shown that $\mathsf{G}(k \to \infty; 0) \sim \gamma k^2$, with γ some constant, is not unphysical. This behaviour has found support in studies concerning stability of the Wigner electron lattice against transverse acoustic (TA) phonon modes (Tozzini and Tosi 1993). For an accurate model

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one-dimensional constant subspace from the representation space for $\chi(\varepsilon = 0)$ and $\chi_0(\varepsilon = 0)$, it is seen that C is well-defined, as in this reduced space both $\chi(\varepsilon = 0)$ and $\chi_0(\varepsilon = 0)$ are negative definite and thus invertible. See, e.g., works by Car, Tosatti, Baroni and Leelaprute (1981) and Mearns and Kohn (1987).

[81] Otherwise the compressibility sum-rule (Pines and Nozières 1966, p. 209), which involves $\chi(k \to 0; \varepsilon = 0)$, and thus $\mathsf{G}(k \to 0; \varepsilon = 0)$ — see Eqs. (133), (134) and (137) —, would be violated.

[82] A consequence of not making distinction between $P^{(0)}[G_0]$ and $P^{(1)}[G]$ — see Subsec. 8.4. We point out that in view of Eqs. (133), (134), (137) and our closing remark in Subsec. 8.4, the $\mathsf{G}(k;0)$-function that we encounter in the present work is *exactly* the $\mathsf{G}(k;0)$-function that has been considered by Holas.

for $\mathsf{G}(k;0)$ see the work by Farid, Heine, Engel and Robertson (1993), and for a recent "diffusion quantum Monte Carlo"-based calculation of $\mathsf{G}(k;0)$ see the paper by Moroni, Ceperley and Senatore (1995). A key element in the work by Holas is his use of $\chi_{\rm td}(\varepsilon)$ (see Eq. (138)), rather than $\chi_{\rm gs}(\varepsilon)$ (see Eq. (136)), in enforcing the energy (frequency) sum-rules concerning the imaginary part of $\chi(\varepsilon)$. Hence, considerations by Holas are (*implicitly*) deeply rooted in the time-dependent DFT and consequently the validity of the treatment by Holas should crucially depend on that of the latter theory for arbitrary values of ε (see Subsubsec. 8.6.2). For typical forms of $\mathsf{G}(k;\varepsilon)$, within various approximation schemes, see the works by Holas, Aravind and Singwi (1979), Devreese, Brosens and Lemmens (1980), Brosens, Devreese and Lemmens (1980) and Brosens and Devreese (1988).

8.7. *Quasi particles; collective charge excitations (Plasmons)*

Let us now consider $\widetilde{\chi}(z)$ in a similar fashion as we did $\widetilde{G}(z)$ in Subsec. 6. We first re-write Eq. (103) as

$$\widetilde{\chi}(z) = -v_c^{-1/2}(I - [v_c^{1/2}\widetilde{P}(z)v_c^{1/2}]^{-1})^{-1}v_c^{-1/2}\,. \tag{139}$$

Here, as in other parts of this work, a (fractional) power of an operator represents an operator that is obtained from the spectral representation of the original operator through raising the eigenvalues (i.e. the spectral weights) to the pertinent power. Let, for instance, $\mathcal{A}$ be a symmetric operator, with $\{\lambda_i\}$ and $\{\mathbf{u}_i\}$ the corresponding eigenvalues and eigenvectors, normalised according to $\mathbf{u}_i^\dagger \cdot \mathbf{u}_j = \delta_{i,j}$. We have $\mathcal{A} = \sum_i \lambda_i \mathbf{u}_i\mathbf{u}_i^\dagger$, so that $\mathcal{A}^\alpha = \sum_i \lambda_i^\alpha \mathbf{u}_i\mathbf{u}_i^\dagger$. The summation over i is symbolic, in that i may be a continuous, or a partially continuous, variable and therefore $\sum_i$ is to be understood as implying also integration. Further, it may occur that in a certain representation, $\mathcal{A}^\alpha$ is *not* an ordinary function but a *distribution* (e.g. involving the δ-function and its derivatives). For this, consider the Fourier representation for v_c in the coordinate representation:

$$v_c(\mathbf{r}-\mathbf{r}') = \int \frac{d^3k}{(2\pi)^3}\,\frac{e^2/\epsilon_0}{\|\mathbf{k}\|^2}\,e^{i\mathbf{k}\cdot\mathbf{r}}e^{-i\mathbf{k}\cdot\mathbf{r}'}\,, \tag{140}$$

where $\int d^3k/[2\pi]^3$ is to be compared with $\sum_i$, $(e^2/\epsilon_0)/\|\mathbf{k}\|^2$ with λ_i and $\exp(i\mathbf{k}\cdot\mathbf{r})$ with $\mathbf{u}_i$.[83] It is obvious that by viewing the RHS of Eq. (140) as an ordinary

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[83] In fact, $\langle\mathbf{r}|\mathbf{u}_{\mathbf{k}} = \exp(i\mathbf{k}\cdot\mathbf{r})$, the usual $\Omega^{-1/2}$ (see Appendix A) is missing because the Fourier-*integral* representation does *not* involve the box normalisation condition.

function, as opposed to a *distribution*, for instance $v_c^{-1/2}$ would be meaningless; already $\langle \mathbf{r}|(v_c)^0|\mathbf{r}'\rangle \equiv \langle \mathbf{r}|I|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}')$, which is a distribution.

The geometric series expansion of $\widetilde{\chi}(z)$ in Eq. (139) in "powers" of $\widetilde{Q}^{-1}(z)$, with

$$\widetilde{Q}(z) := [v_c^{1/2}\widetilde{P}(z)v_c^{1/2}] \tag{141}$$

diverges when

$$\det(I - \widetilde{Q}^{-1}(z)) = 0\,. \tag{142}$$

This eqnation is similar to that in Eq. (54). As we shall see, solutions of this equation, or the equation obtained from it through the process of analytic continuation of $\widetilde{Q}^{-1}(z)$ into a no-physical RS, are of physical significance — they correspond to excitations of the charge density in the N-electron system, i.e. to charge-neutral excitations. This is explicit in the Lehmann-type representation for $\chi(\varepsilon)$ in Eq. (100).

Solutions of Eq. (142) are related to eigenvalues of the following eigenproblem in a way that will become clear shortly:

$$\widetilde{Q}(z)\widetilde{\xi}_s(z) = \widetilde{D}_s(z)\widetilde{\xi}_s(z)\,, \tag{143}$$

$$\widetilde{\zeta}_s^{\dagger}(z)\widetilde{Q}(z) = \widetilde{D}_s(z)\widetilde{\zeta}_s^{\dagger}(z) \iff \widetilde{Q}^{\dagger}(z)\widetilde{\zeta}_s(z) = \widetilde{D}_s^{*}(z)\widetilde{\zeta}_s(z)\,. \tag{144}$$

Here $\widetilde{\xi}_s(z)$ and $\widetilde{\zeta}_s(z)$ are, respectively, the *right* and *left* eigenfunctions of $\widetilde{Q}(z)$ corresponding to eigenvalue $\widetilde{D}_s(z)$ (we assume that these eigenfunctions have been appropriately ordered — see Footnote 30). In cases where $\widetilde{D}_s(z) \neq \widetilde{D}_{s'}(z)$, these eigenfunctions are bi-orthogonal and can be normalised, i.e. $\langle \widetilde{\xi}_s(z), \widetilde{\zeta}_{s'}(z)\rangle = \delta_{s,s'}$. In cases of degeneracy, a Gram-Schmidt orthogonalisation procedure can be applied to achieve that the latter property holds for *all* $\widetilde{\xi}_s(z)$ and $\widetilde{\zeta}_{s'}(z)$. For some relevant further details see text following Eq. (59) above.

Since for a general z, $\widetilde{Q}(z)$ is *non*-Hermitian (it holds however that $\widetilde{Q}(\mathbf{r},\mathbf{r}';z) = \widetilde{Q}(\mathbf{r}',\mathbf{r};z)$), the two sets of left and right eigenfunctions of $\widetilde{Q}(z)$ do *not* coincide, nor are the eigenfunctions within each of the two sets orthogonal. The spectral representation of $\widetilde{Q}(z)$ should therefore be a bi-orthonormal representation (Morse and Feshbach 1953, pp. 884–886, Farid, Engel, Daling and van Haeringen 1991) as follows

$$\widetilde{Q}(\mathbf{r},\mathbf{r}';z) = \sum_s \widetilde{D}_s(z)\widetilde{\xi}_s(\mathbf{r};z)\widetilde{\zeta}_s^{*}(\mathbf{r}';z)\,. \tag{145}$$

By completeness, i.e. $\sum_s \widetilde{\xi}_s(z)\widetilde{\zeta}_s^\dagger(z) = I$, we can write (see Eq. (139))

$$\widetilde{\chi}(\mathbf{r},\mathbf{r}';z) = 2\sum_s \frac{\overline{\widetilde{\xi}}_s(\mathbf{r};z)\overline{\widetilde{\zeta}}{}^*_s(\mathbf{r}';z)}{\overline{\widetilde{D}}_s(z)}\,, \tag{146}$$

where

$$\overline{\widetilde{\xi}}_s(z) := v_c^{-1/2}\widetilde{\xi}_s(z)\,, \quad \overline{\widetilde{\zeta}}_s(z) := (v_c^{-1/2})^\dagger\widetilde{\zeta}_s(z) \tag{147}$$

and

$$\overline{\widetilde{D}}_s(z) := 2\left(1 - \frac{1}{\widetilde{D}_s(z)}\right)\,. \tag{148}$$

From the above representation we observe that the singular points of $\widetilde{\chi}(z)$ coincide with solutions of the following equivalent equations

$$\overline{\widetilde{D}}_s(z) = 0 \iff \widetilde{D}_s(z) = 1\,. \tag{149}$$

In view of Eq. (145) and the completeness relation, $\sum_s \widetilde{\xi}_s(z)\widetilde{\zeta}_s^\dagger(z) = I$, it is obvious that the solutions of the second of the above equations indeed satisfy Eq. (142). We note that, similar to the case that we have considered in Sec. 6, here there are some symmetry relations, and properties associated with these, that can be readily verified: We have $\widetilde{P}(\mathbf{r},\mathbf{r}';z) = \widetilde{P}(\mathbf{r}',\mathbf{r};z)$ and $\widetilde{P}(z^*) = \widetilde{P}^\dagger(z)$ — see Eqs. (105) and (110) —, from which, making use of $\langle\mathbf{r}|\widetilde{P}^\dagger(z)|\mathbf{r}'\rangle \equiv \langle\mathbf{r}'|\widetilde{P}(z)|\mathbf{r}\rangle^*$, it follows that

$$\widetilde{\zeta}_s(\mathbf{r};z) = \widetilde{\xi}_s(\mathbf{r};z^*)\,; \quad \widetilde{\xi}_s(\mathbf{r};z) = \widetilde{\zeta}_s(\mathbf{r};z^*)\,; \quad \widetilde{D}_s(z^*) = \widetilde{D}_s^*(z)\,, \quad \mathrm{Im}(z) \neq 0\,. \tag{150}$$

Also, on account of the time-reversal symmetry (see Subsec. 4.4), for every s there exists an $\overline{s}$ for which $\widetilde{D}_{\overline{s}}(z) = \widetilde{D}_s(z)$, $\widetilde{\xi}_{\overline{s}}(\mathbf{r};z) = e^{i\theta_s}\widetilde{\zeta}_s^*(\mathbf{r};z)$ and $\widetilde{\zeta}_{\overline{s}}(\mathbf{r};z) = e^{i\theta_s}\widetilde{\xi}_s^*(\mathbf{r};z)$ hold, with θ_s some real constant, independent of $\mathbf{r}$. From these results it follows directly that $\widetilde{\xi}_{\overline{s}}(\mathbf{r};z) = e^{i\theta_s}\widetilde{\xi}_s(\mathbf{r};z^*)$ and $\widetilde{\zeta}_{\overline{s}}(\mathbf{r};z) = e^{i\theta_s}\widetilde{\zeta}_s(\mathbf{r};z^*)$.

Concerning the requirement of *explicit* orthogonalisation of $\widetilde{\xi}_s(z)$ and $\widetilde{\zeta}_{s'}(z)$ when $\widetilde{D}_s(z) = \widetilde{D}_{s'}(z)$ for $s \neq s'$, such as is the case when $s' = \overline{s}$ (see above), we mention that this orthogonality is automatically taken care of if the sets $\{\widetilde{\xi}_s\}$, $\{\widetilde{\zeta}_s\}$ are chosen to be simultaneously bases of the unitary irreducible representations of the underlying symmetry group of the Hamiltonian of the system: when the degenerate *right* and *left* eigenfunctions $\widetilde{\xi}_s(z)$ and $\widetilde{\zeta}_{s'}(z)$

belong to *different* unitary irreducible representation of the mentioned group, the two functions are orthogonal (Cornwell 1984, pp. 81–83).

Some remark concerning the asymptotic behaviour of the above quantities for $|z| \to \infty$ is in place. From Eqs. (117) and (118) it follows that $\widetilde{P}(z)$ diminishes like $1/z^2$ for large $|z|$. Normalisation of the eigenfunctions implies that for the Eqs. (143), (144) to be valid in this asymptotic regime, it is necessary that $\widetilde{D}_s(z) \sim' 1/z^2$ for $|z| \to \infty$. From Eq. (148) we deduce that therefore $\widetilde{\widetilde{D}}_s(z) \sim' z^2$. Substituting this result in the representation in Eq. (146) we obtain, consistently (since the functions in the numerator are normalised), that indeed $\widetilde{\chi}(z)$ approaches zero like $1/z^2$ (see Eqs. (110) and (118)).

When $\widetilde{\widetilde{D}}_s(z_i) = 0$, we have in addition $\widetilde{\widetilde{D}}_s(-z_i) = 0$. This follows from the equivalence between solutions of Eqs. (142) and (149), and the fact that $\widetilde{P}(z)$, and therefore $\widetilde{Q}(z)$, is an even function of z. Thus near each z_i, $\widetilde{\widetilde{D}}_s(z) \sim' z^2 - z_i^2$, in conformity with the Lehmann-type representation in Eq. (110).

Concerning the physical significance of the solutions of Eq. (142) (or of Eq. (143)), $\{z_i\}$, and the corresponding eigenfunctions $\widetilde{\xi}_s(z_i)$, we mention that according to Eq. (96), $\chi(\mathbf{r}t, \mathbf{r}'t')$ describes, to linear order, the change in the density of the electrons at the space-time point $\mathbf{r}t$ in response to a change in the local external potential at the space-time point $\mathbf{r}'t'$. Equivalently, we have $\delta\widetilde{n}(z) = \widetilde{\chi}(z)\delta\widetilde{\varphi}(z)$. The closer the "energy" z to energies at which $\widetilde{\chi}(z)$ is singular, the smaller the amplitude of the required external potential needs to be in order to bring about oscillations of a given amplitude in the electronic distribution of the system, so much so that at the singularity z_i, the charge density undergoes self-sustained oscillations, without the agency of an external potential. Self-sustained charge oscillations in an electronic system are termed *plasmons*. Thus solutions of Eq. (142) are plasmon energies. Traditionally, the solutions of $\det[\epsilon(\varepsilon)] = 0$ are considered to signify these energies. Since according to Eq. (95), $\widetilde{\epsilon}^{-1}(z) = I + v_c\widetilde{\chi}(z)$, and since v_c is positive definite, it follows that $\det[\widetilde{\epsilon}^{-1}(z)] \equiv 1/\det[\widetilde{\epsilon}(z)] = \det[I + v_c^{1/2}\widetilde{\chi}(z)v_c^{1/2}]$, so that indeed $\det[\widetilde{\epsilon}(z)] = 0 \iff 1/\det[\widetilde{\chi}(z)] = 0 \iff \widetilde{\widetilde{D}}_s(z) = 0$ for some s.

From $\delta\widetilde{n}(z) = \widetilde{\chi}(z)\delta\widetilde{\varphi}(z)$ it follows that at the possible plasmon energies $\{z_i^{pl}\}$ we must have $\widetilde{\chi}^{-1}(z_i^{pl})\delta\widetilde{n}(z_i^{pl}) = 0$, that is, in the case of non-degeneracy $\delta\widetilde{n}(z_i^{pl})$ is a multiple of the *right* eigenvector of $\widetilde{\chi}(z)$ — note that the left and right eigenvectors of an operator and of its inverse are identical —; in the case of degeneracy, $\delta n(\varepsilon_i^{pl})$ is a linear superposition of the degenerate right eigenstates. It should be mentioned that such analysis as the above, aimed at the determination of the resonant energies of a system, is based on a linear-response theory and therefore *cannot* determine the amplitudes $\delta\tilde{n}(z_i^{pl})$ of the charge excitations. However, for the linear-response theory to be applicable, these amplitudes must be small — for otherwise non-linear effects (i.e. mode-mode coupling effects) cannot be neglected. In reality it is owing to these effects that amplitudes of the excitation modes are bounded.

It is interesting to enquire as to the origin of the apparent privileged role that the *right* eigenfunction, as opposed to the *left* eigenfunctions, of $\tilde{\chi}$ play in the context of plasmon excitations; the same may be enquired with regard to the right eigenfunctions of $\tilde{\mathcal{H}}_{qp}(z)$, which play the role of the QP "wavefunctions" — see Eq. (58). The origin of this bias lies in the fact that Eq. (149) has either real-valued solutions or it has *no* solution. This condition is identical with that which we have encountered in our discussions concerning QPs and their corresponding energies in Sec. 6. Here, owing to the reflection property $\tilde{D}_s(z^*) = \tilde{D}_s^*(z)$, $\tilde{D}_s(z_i) = 1$ for some *complex-valued* z_i implies that also $\tilde{D}_s(z_i^*) = 1$. That is, the possible complex-valued solutions of $\tilde{D}_s(z) = 1$, if any, must occur in complex-conjugate pairs. This is in violation of the causality principle — recall that $\chi(\mathbf{r}t, \mathbf{r}'t')$ is defined as the GS expectation value of a *time-ordered* product of the density-fluctuation operators. Therefore, the energies of the *damped* plasmon excitations, if any, must lie on a non-physical RS of the z-plane; with $\tilde{\tilde{D}}_s(z)$ an analytic continuation of $\tilde{D}_s(z)$ into a non-physical sheet (see Subsec. 2.2), the complex-valued solutions satisfy $\tilde{\tilde{D}}_s(z) = 1$. For the real energy ε_i to be a solution of $\tilde{D}_s(z) = 1$, it is necessary that $\mathrm{Im}\tilde{D}_s(\varepsilon_i) = 0$. For such an ε_i, $\tilde{\chi}(\varepsilon_i \pm i\eta) \equiv \chi(\varepsilon_i)$ (see Eq. (111)) is Hermitian, so that the sets of *left* and *right* eigenfunctions of $\tilde{\chi}(z)$ coincide and therefore there is no bias. Let us now disregard the fact that $\tilde{D}_s(z) = 1$ *cannot* have complex-valued solutions, and thus assume that z_i and z_i^* were two complex conjugate solutions of this equation. Because of the properties in Eq. (150), it follows that the *right* eigenfunction of $\tilde{\chi}(z)$ at z_i, i.e. $\tilde{\tilde{\xi}}_s(z_i)$ — see Eqs. (143) and (147) —, is identical with the *left* eigenfunction of $\tilde{\chi}(z)$ at z_i^*, i.e. $\tilde{\tilde{\zeta}}_s(z_i^*)$ — see Eqs. (144) and (147). Thus even in this hypothetical case, corresponding to complex-valued solutions for $\tilde{D}_s(z) = 1$, there is *no* privileged position taken by the *right* eigenfunctions of $\tilde{\chi}(z)$.

In closing this section, we mention that the technique of analytic continuation of $\tilde{\chi}(z)$ into a non-physical RS (Farid, Engel, Daling and van Haeringen 1991) has been employed for obtaining the complex plasmon energies in real semiconducting materials (Daling, van Haeringen and Farid 1991, 1992). The analytically continued response functions evaluated on the real energy axis yield very reliable results, including those that can be experimentally probed, such as the electron loss function or the dynamical electron structure factor. This approach has been successfully employed for obtaining dynamical response functions of semiconductors (Daling, van Haeringen and Farid 1991, 1992), metals (Maddocks, Godby and Needs 1994a, 1994b) and cuprate superconductors (Dadachanji, Godby, Needs and Littlewood 1995).

8.8. *Pair-correlation functions*

From Eqs (110), (111) and (112) — or from Eq. (100), through applying $1/(x-x_0 \pm i\eta) = \mathcal{P}\,(1/(x-x_0)) \mp i\pi\delta(x-x_0)$, with $\eta \downarrow 0$ — it follows that for $\chi''(\varepsilon)$ in $\chi'(\varepsilon) + i\chi''(\varepsilon) \equiv \chi(\varepsilon)$

$$\chi''(\mathbf{r},\mathbf{r}';\varepsilon) = -2\pi \sum_s \varrho_s(\mathbf{r})\varrho_s^*(\mathbf{r}')\{\delta(\varepsilon - e_s) + \delta(\varepsilon + e_s)\} \tag{151}$$

holds. Since $e_s > 0$ for *all* $s \neq 0$ (see Eq. (102)), from Eq. (151) the following expressions are readily obtained

$$\begin{aligned}\frac{-1}{\pi}\int_0^\infty d\varepsilon\chi''(\mathbf{r},\mathbf{r}';\varepsilon) &= 2\sum_s \varrho_s(\mathbf{r})\varrho_s^*(\mathbf{r}') \\ &= 2\langle\Psi_{N,0}|\widehat{n}(\mathbf{r})\widehat{n}(\mathbf{r}')|\Psi_{N,0}\rangle - \frac{1}{2}n(\mathbf{r})n(\mathbf{r}')\,;\end{aligned} \tag{152}$$

$$\begin{aligned}\frac{-2}{\pi}\int_0^\infty d\varepsilon\varepsilon\chi''(\mathbf{r},\mathbf{r}';\varepsilon) &= 4\sum_s e_s\varrho_s(\mathbf{r})\varrho_s^*(\mathbf{r}') \\ &= \lim_{|\varepsilon|\to\infty} \varepsilon^2\chi(\mathbf{r},\mathbf{r}';\varepsilon) =: \chi_{\infty_2}(\mathbf{r},\mathbf{r}')\,.\end{aligned} \tag{153}$$

The LHSs of Eqs. (152) and (153) are the zeroth and first energy ("*f*requency") moments of $\chi''(\varepsilon)$, respectively. In fact through combining Eqs. (153) and (122), one arrives at the well-known *f*-sum rule (Nozières 1964, Johnson 1974, Schülke 1983, Taut 1985a,b, Engel and Farid 1993) for the density-density correlation function.

One interesting aspect of the result in Eq. (152) is the following. The static pair-correlation function is defined as follows

$$g(\mathbf{r},\mathbf{r}') := \frac{1}{N(N-1)}\{2\langle\Psi_{N,0}|\widehat{n}(\mathbf{r})\widehat{n}(\mathbf{r}')|\Psi_{N,0}\rangle - n(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\}\,. \tag{154}$$

Making use of Eq. (101) one obtains

$$\begin{aligned} g(\mathbf{r},\mathbf{r}') &= \frac{1}{N(N-1)}\left\{2\sum_s \varrho_s(\mathbf{r})\varrho_s^*(\mathbf{r}') + \frac{1}{2}n(\mathbf{r})n(\mathbf{r}') - n(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\right\} \\ &= \frac{1}{N(N-1)}\left\{\frac{-1}{\pi}\int_0^\infty d\varepsilon\chi''(\mathbf{r},\mathbf{r}';\varepsilon) + \frac{1}{2}n(\mathbf{r})n(\mathbf{r}') - n(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\right\}. \end{aligned} \tag{155}$$

Thus the zeroth energy moment of $\chi''(\mathbf{r},\mathbf{r}';\varepsilon)$ is closely related to the electronic pair-correlation function $g(\mathbf{r},\mathbf{r}')$.

For systems in the thermodynamic limit (below signified by means of "$\cong$"), the quantity of interest is $\overline{g}(\mathbf{r},\mathbf{r}') := \Omega^2 g(\mathbf{r},\mathbf{r}')$, for which

$$\overline{g}(\mathbf{r},\mathbf{r}') \cong \frac{1}{\overline{n}^2}\{2\langle\Psi_{N,0}|\widehat{n}(\mathbf{r})\widehat{n}(\mathbf{r}')|\Psi_{N,0}\rangle - n(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\} \tag{156}$$

holds, where $\overline{n} := N/\Omega$ ($\equiv \mathsf{C}$ — see Subsec. 2.4) is the average density of electrons, or concentration. We shall have occasion to use

$$2\sum_s \varrho_s(\mathbf{r})\varrho_s^*(\mathbf{r}') = \frac{N(N-1)}{\Omega^2}g(\mathbf{r},\mathbf{r}') - \frac{1}{2}n(\mathbf{r})n(\mathbf{r}') + n(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}'), \tag{157}$$

which follows from Eqs. (152) and (154).

For systems without off-diagonal long-range order, ODLRO (Reichl 1980, pp. 202–205), i.e. those involving no superconductivity or superfluidity, one has[84]

$$\lim_{\|\mathbf{r}-\mathbf{r}'\|\to\infty}\langle\Psi_{N,0}|\widehat{n}(\mathbf{r})\widehat{n}(\mathbf{r}')|\Psi_{N,0}\rangle = \frac{1}{2}n(\mathbf{r})n(\mathbf{r}'), \tag{158}$$

so that the correlation function

$$\overline{\overline{g}}(\mathbf{r},\mathbf{r}') := \frac{\overline{n}^2}{n(\mathbf{r})n(\mathbf{r}')}\,\overline{g}(\mathbf{r},\mathbf{r}') \tag{159}$$

pertaining to such systems has the property that $\overline{\overline{g}}(\mathbf{r},\mathbf{r}') \to 1$ when $\|\mathbf{r}-\mathbf{r}'\| \to \infty$. In the literature there are at least two different pair-correlation functions in use. One of these is the van Hove (1954a,b) pair-correlation function g_{vH}

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[84] Here we have summed over the internal spin degree of freedom, without which the 1/2 on the RHS would have been 1/4.

which can be shown to coincide with g in Eq. (154):

$$g_{vH}(\mathbf{r},\mathbf{r}') := \frac{2}{N(N-1)} \langle \Psi_{N,0} | \widehat{\psi}^{\dagger}(\mathbf{r}') \widehat{\psi}^{\dagger}(\mathbf{r}) \widehat{\psi}(\mathbf{r}) \widehat{\psi}(\mathbf{r}') | \Psi_{N,0} \rangle \equiv g(\mathbf{r},\mathbf{r}'). \qquad (160)$$

Concerning the second, within the framework of the DFT one encounters a pair-correlation function whose "coupling-constant integration" (the coupling constant being e^2, the electron-charge squared) yields the exchange-correlation energy functional (Langreth and Perdew 1975, Gunnarsson and Lundqvist 1976, Harris 1984).[85] This pair-correlation function coincides with $\overline{\overline{g}}(\mathbf{r},\mathbf{r}')$ given in Eq. (159).

8.9. *The continued-fraction expansion and its physical significance*

As a typical example of functions with "branch-cut discontinuity", we take $\widetilde{\chi}(z)$. From the Lehmann-type representation in Eq. (100), one immediately obtains the following spectral representation (see Eqs. (111) and (112) for χ'')

$$\chi(\varepsilon) = \frac{-1}{\pi} \int_0^{+\infty} d\varepsilon' \left\{ \frac{1}{\varepsilon - \varepsilon' + i\eta} - \frac{1}{\varepsilon + \varepsilon' - i\eta} \right\} \chi''(\varepsilon'). \qquad (161)$$

Suppose that for $\varepsilon > 0$, $\chi''(\varepsilon)$ differs from zero only in the finite interval $[\varepsilon_{\min}, \varepsilon_{\max}]$ with $\varepsilon_{\min}, \varepsilon_{\max} > 0$, so that the ε'-integral in Eq. (161) can be written as one over this finite interval. Suppose further that $\varepsilon_0 \in [\varepsilon_{\min}, \varepsilon_{\max}]$ and let ε be chosen such that for $\varepsilon' \in [\varepsilon_{\min}, \varepsilon_{\max}]$, $|(\varepsilon' - \varepsilon_0)/(\varepsilon \pm \varepsilon_0)| < 1$. When these conditions are fulfilled, one has the following exact result

$$\chi(\varepsilon) = \frac{-1}{\pi} \sum_{m=0}^{\infty} \left\{ \frac{1}{(\varepsilon - \varepsilon_0)^{m+1}} - \frac{(-1)^m}{(\varepsilon + \varepsilon_0)^{m+1}} \right\}$$
$$\times \sum_{l=0}^{m} \binom{m}{l} (-\varepsilon_0)^{m-l} \int_{\varepsilon_{\min}}^{\varepsilon_{\max}} d\varepsilon' \varepsilon'^{l} \chi''(\varepsilon'), \qquad (162)$$

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[85] The system to which this pair-correlation function pertains is one in which a coupling-constant-dependent external local potential ensures that for all values of the coupling constant between zero and the physical value of e^2, the GS charge density is identical to that of the *fully*-interacting system.

which signifies the importance of the energy moments[86] of the branch-cut discontinuity of $\widetilde{\chi}(z)$.[87] From Eq. (162) it can directly be seen that in the limit of $|\varepsilon| \gg \varepsilon_0$, only the *odd* central energy moments of $\chi''(\varepsilon)$ contribute to $\chi(\varepsilon)$. The most prominent (from the point of view of the asymptotic behaviour of $\chi(\varepsilon)$ for $|\varepsilon| \to \infty$) *central* energy moment of $\chi''(\varepsilon)$ is thus the first-order moment. Correctness of the zeroth- *and* first-order moments of $\chi''(\varepsilon)$ guarantee correctness of this first-order *central* energy moment. The first-order moment of in particular $\chi''(\varepsilon)$ is designated as the f-sum, and a relationship between this f-sum and some GS properties is thus referred to as the "f-sum rule" (Nozières 1964, pp. 45–50, Johnson 1974, Schülke 1983, Taut 1985a,b; see text following Eq. (153) above). The so-called plasmon-pole models for the density-density correlation function, or the dielectric response function (Hybertsen and Louie 1985, 1986, 1988, von der Linden and Horsch 1988, Engel and Farid 1993), are simplified expressions for $\chi''(\varepsilon)$ (or some associated function, such as $\epsilon^{-1''}(\varepsilon)$ — see Subsec. 7.5) which *in principlc* guarantee satisfaction of the f-sum rule. In Subsec. 8.10 we shall discuss one of the most reliable of the plasmon-pole models concerning $\chi(\varepsilon)$ (Engel and Farid 1993).

Having explicitly considered the relevance of the energy moments of $\chi''(\varepsilon)$, we now examine the significance of the encrgy moments for a more general operator and within a somewhat broader context. To this end, let $\widetilde{f}(z)$ be analytic everywhere on the complex z-plane, except along the real interval $[\varepsilon_{\min}, \varepsilon_{\max}]$. With

$$g(\varepsilon) := \frac{1}{2i}\{\widetilde{f}(\varepsilon + i\eta) - \widetilde{f}(\varepsilon - i\eta)\}\,, \tag{163}$$

to be compared with $\chi''(\varepsilon)$, nsing the Cauchy theorem (Titchmarsh 1939, p. 102) one can show that

$$\widetilde{f}(z) = \frac{1}{\pi}\int_{\varepsilon_{\min}}^{\varepsilon_{\max}} d\varepsilon'\, \frac{g(\varepsilon')}{\varepsilon' - z}\,. \tag{164}$$

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[86] According to Kubo and Tomita (1954), "the moment method" is introduced by Broer (1943), Van Vleck (1948) and Pryce and Stevens (1951), and "is the most common and basic method used so far for the discussions of the line shapes of magnetic resonance absorption." For specific applications see works by Kubo and Tomita (1954), Harris and Lange (1967), Haydock (1980, pp. 289 and 290) and Nolting and Oleś (1987).

[87] The second sum on the RHS of Eq. (162) is in fact nothing but the mth *central* moment of $\chi''(\varepsilon)$ — *ccntral* with respect to ε_0. We note that moments expansion in terms of central moments has superior convergence property as compared to that in terms of usual moments, which are the "central moments" with respect to $\varepsilon_0 = 0$; the usual moments in general rapidly grow with the increasing order of moments.

Now provided $g(\varepsilon)$ does *not* change sign for $\varepsilon \in (\varepsilon_{\min}, \varepsilon_{\max})$, $\widetilde{f}(z)$ can be represented in terms of a *continued fraction* (Ince 1926, pp. 178–185) of infinite order (Cheney 1966, p. 186).[88] It can be shown that truncating this expansion at a finite order M, yields a function $\widetilde{f}_M(z)$ which can be represented in the following form (Cheney 1966, p. 186)

$$\widetilde{f}_M(z) = \frac{-1}{\pi} \sum_{m=1}^{M} \frac{w_m}{z - \varepsilon_m}, \tag{165}$$

where $\{w_m | m = 1, 2, \ldots, M\}$ is the set of some well-specified coefficients, and $\{\varepsilon_m | m = 1, 2, \ldots, M\}$ that of zeros of a polynomial of order M, obtained from a recurrence relation (which generates *orthogonal* polynomials) whose coefficients are *functionals* of $g(\varepsilon)$ (Szegö 1967, Hochstrasser, U.W., in Abramowitz and Stegun 1972, Ch. 22). We point out that $\varepsilon_{\min} < \varepsilon_m < \varepsilon_{\max}$ for *all* values of m. Now we define

$$g_M(\varepsilon) := \frac{1}{2i} \{\widetilde{f}_M(\varepsilon + i\eta) - \widetilde{f}_M(\varepsilon - i\eta)\}. \tag{166}$$

From Eq. (163) the parallel between $g_M(\varepsilon)$ and $g(\varepsilon)$ is apparent. Two interesting properties of $\widetilde{f}_M(z)$ are that: (i) for $\mathrm{Im}(z) \neq 0$, $\widetilde{f}_M(z)$ converges to $\widetilde{f}(z)$ for increasing M and (ii) for a *polynomial* $h(\varepsilon)$ of degree not larger than $2M - 1$, the following is exact:

$$\begin{aligned} \int_{\varepsilon_{\min}}^{\varepsilon_{\max}} d\varepsilon' g(\varepsilon') h(\varepsilon') &= \sum_{m=1}^{M} w_m h(\varepsilon_m) \\ &\equiv \int_{\varepsilon_{\min}}^{\varepsilon_{\max}} d\varepsilon' g_M(\varepsilon') h(\varepsilon'). \end{aligned} \tag{167}$$

The first of these relations is a Gaussian quadrature rule (Stoer and Bulirsch 1980) for the general weight function $g(\varepsilon)$.[89] From Eq. (167) we observe that as

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[88] The restriction on $g(\varepsilon)$ in having a definite sign (positive or negative), is imposed for avoiding semi-definite "norms" which in the process of evaluating the coefficients of the continued-fraction expansion may give rise to zero denominators. For treatment of cases where $g(\varepsilon)$ changes sign, we refer the reader to the paper by Engel and Farid (1992).

[89] Orthogonal polynomials are "orthogonal" over some well-specified interval *and* with respect to some well-specified weight function. For instance, the Chebyshev polynomials $T_m(x)$, $m = 0, 1, \ldots$, are defined over $[-1, 1]$ and are mutually orthogonal with respect to the weight function $(1 - x^2)^{-1/2}$, $\int_{-1}^{+1} dx (1 - x^2)^{-1/2} T_m(x)\, T_n(x) = \delta_{m,n}$. See Hochstrasser, U.W., in (Abramowitz and Stegun 1972, Ch. 22).

far as integrals of polynomials of degree not higher than $2M-1$ are concerned, the weight function g_M is equivalent to g. In other words, the first $2M-1$ energy (i.e. ε) moments of $g_M(\varepsilon)$ and $g(\varepsilon)$ *are* identical. Returning to $\chi''(\varepsilon)$, as far as the energy moments of this function up to some finite order are concerned, $\chi''(\varepsilon)$ can be represented in terms of a discrete sum over a *finite* number of δ-functions along the real energy axis (*c.f.* Eq. (165) in conjunction with Eq. (166), taking $z = \varepsilon \pm i\eta$ with $\eta \downarrow 0$); under the conditions for which Eq. (162) is valid, such a representation for $\chi''(\varepsilon)$ can yield very accurate $\chi(\varepsilon)$, even for a small M. Although in this way the behaviour of $\chi''(\varepsilon)$ aloug the real ε-axis may not be correctly represented (recall that for systems in the thermodynamic limit, there are branch-cut discontinuities along the real energy axis), nonetheless the energy moments of $\chi''(\varepsilon)$ up to some finite order *are* exactly reproduced. We shall not enter into details here, but mention that through introduction of a so-called terminating function (Nex 1985), or through displacement of the branch cuts form the real axis into the complex plane (Engel, Farid, Nex and March 1991),[90] it is possible to construct a $\chi(\varepsilon)$ that has the correct behaviour on the real axis. These techniques have been successfully applied in obtaining the plasmon energy bands of inhomogeneous systems (Engel, Farid, Nex and March 1991, Engel and Farid 1992); for a review see the paper by Farid, Engel, Daling and van Haeringen (1994).

8.10. *A plasmon-pole approximation*

Consider the following function of z (Engel and Farid 1993)

$$\widetilde{\chi}_{pp}(z) := (z^2\chi_{\infty_2}^{-1} + \chi^{-1}(0))^{-1}\,; \tag{168}$$

for χ_{∞_2} see Eqs. (118), (122), (123) and (128) — see also Subsec. 8.5. Clearly, $\widetilde{\chi}_{pp}(z)$ has the property that at two limits $z \to 0$ and $|z| \to \infty$ yields the results corresponding to the exact χ. In particular because of the latter, $\chi_{pp}(\varepsilon)$ satisfies the f-fum rule (see Eq. (153) and Subsec. 8.9). Certain approximate expressions that yield the "exact" static χ in the static limit and moreover satisfy the f-sum rule are referred to as "plasmon-pole" (pp) models for χ. In the course of years a number of such models have been proposed and applied. The above model has a number of advantages that are not shared by other models. For details we refer the reader to the original work.

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[90] Branch cuts, contrary to branch points, can be displaced. In other words, the precise location of branch cuts of an analytic function is a matter of convention.

It is important to point out that for systems in which $w(\mathbf{r},\mathbf{r}') \equiv 0$, $\chi_0(\varepsilon)$, or $P_0(\varepsilon;[G_{KS}])$, has the property (see Subsec. 8.5) $\chi_{0;\infty_2} \equiv \chi_{\infty_2}$, so that $\widetilde{\chi}_{pp}(z)$ in Eq. (168) is manifestly *fully* determined in terms of the ingredients of the GS DFT (for $\chi(0)$ see Eqs. (133) and (134) above).

The plasmon-pole model in Eq. (168) can be expressed in terms of the eigenfunctions and eigenvalues of the following generalised eigenvalue problem (Engel and Farid 1993)

$$\chi(0)\zeta_i = -\frac{1}{\mathsf{e}_i^2}\chi_{\infty_2}\zeta_i \tag{169}$$

subject to the normalisation condition

$$\zeta_i^\dagger \chi_{\infty_2}\zeta_j = \delta_{i,j}\,. \tag{170}$$

It can easily be verified that $\widetilde{\chi}(z)$ has the following spectral representation

$$\widetilde{\chi}_{pp}(z) = 4\sum_i \mathsf{e}_i \frac{\varsigma_i\varsigma_i^\dagger}{z^2-\mathsf{e}_i^2}\,, \tag{171}$$

which has the form of the exact Lehmann-type representation in Eq. (110). In Eq. (171),

$$\varsigma_i := \frac{1}{2\mathsf{e}_i^{1/2}}\chi_{\infty_2}\zeta_i\,. \tag{172}$$

Since both $\chi(0)$ and $-\chi_{\infty_2}$ are negative semi-definite (see text following Eq. (116)), e_i is indeed non-negative (similar to e_s in Eq. (102) above), so that the square root in Eq. (172) is real-valued. The dynamical part of the screened-interaction function associated with $\widetilde{\chi}_{pp}(z)$, i.e. $\widetilde{\overline{W}}_{pp}(z)$ is easily obtained (see Eq. (175) below). Using the fact that $\chi(\varepsilon) \equiv \lim_{\eta\downarrow 0}\widetilde{\chi}(\varepsilon \pm i\eta)$ — Eq. (111) —, depending on whether $\varepsilon > 0$ or $\varepsilon < 0$, from Eq. (171) we readily obtain

$$\chi_{pp}(\mathbf{r},\mathbf{r}';\varepsilon) = 2\sum_i \varsigma_i(\mathbf{r})\varsigma_i^*(\mathbf{r}')\left\{\frac{1}{\varepsilon-\mathsf{e}_i+i\eta} - \frac{1}{\varepsilon+\mathsf{e}_i-i\eta}\right\}. \tag{173}$$

The similarity between this expression and the Lehmann-type representation in Eq. (100) is apparent. Plausibility arguments, supported by numerical as well as experimental results (Engel and Farid 1993), suggest that $\{\mathsf{e}_i\} \leftrightarrow \{\mathsf{e}_\ell(\mathbf{k})\}$, with $\mathbf{k} \in$ 1BZ, to a high degree of accuracy should coincide with positions of peaks in the energy-loss spectra for (periodic) crystals, i.e. with the plasmon band energies.

9. The *GW* Approximation for The Self-Energy

A physically appealing approximation for Σ that can be derived both from the coupled set of equations in Eqs. (90)–(93) and from the perturbation expansion for Σ in terms of the dynamic screened interaction function W, is the dynamically screened exchange SE, also referred to as the *GW* self-energy (see Fig. 12(b)). What is meant by the *GW* self-energy operator, Σ^{GW}, concerns the first-order contribution to $(\Sigma - \hbar^{-1} v_H)$ in a perturbation expansion in terms W — see Subsec. 7.6. The first-order SE diagrams are all skeleton so that at the level of the first-order perturbation expansion, $\Sigma^{\{0\}}[F]$ and $\Sigma^{\{1\}}[F]$ are identical (see Subsec. 7.6). Thus $\Sigma^{GW}[F]$ does not need to be further specified by means of superscripts $\{0\}$ and $\{1\}$. Therefore, the only ambiguity in the calculation of $\Sigma^{GW}[F]$ arises from the freedom in the choice for F. In this Section we choose F to coincide with the *exact* G, so that many of the expressions that we present below involve the Lehmann amplitudes and energies, $f_s(\mathbf{r})$ and ε_s, defined in Eqs. (12) and (13), respectively, in terms of which G is represented in Eq. (11). Where appropriate, we shall indicate how the pertinent expressions corresponding to $\Sigma^{GW}[G]$ are modified in consequence of replacing G in $\Sigma^{GW}[G]$ by *some* G_0. Thus the choice $F = G$ enables us to enquire into the aspects of a G_0 for which $\Sigma^{GW}[G_0]$ as closely as possible reproduces certain results that are specific to $\Sigma^{GW}[G]$ (see Subsecs. 9.6 and 9.7). We should like to emphasise that Σ^{GW} being an *approximation* to $(\Sigma - \hbar^{-1} v_H)$, there is no *a priori* reason to believe that results obtained from $\Sigma^{GW}[G]$ should necessarily be in a better *quantitative* agreement with the experimental results than those obtained from $\Sigma^{GW}[G_0]$ for *some* G_0 (say the one pertaining to the KS Hamiltonian within the LDA for the exchange-correlation potential) — see Subsec. 9.12.

9.1. *Some historical background*

The *GW* scheme was first put forward by Hedin (1965) as the leading-order term in a series expansion for the SE operator in terms of the dynamically-screened interaction function W (Hubbard 1957) (see the works by DuBois (1959a), (1959b)); this expansion was derived as a means for a systematic decomposition of the coupled set of equations (Hedin 1965) which we have presented in Subsec. 7.5 (Eqs. (90)–(93)). Hedin's approach is based on the Schwinger variational principle (Schwinger 1951a,b,c; see Martin and Schwinger 1959) which in turn is a differential form of the Feynman (1948) principle

— what has now become Feynman's path-integral formalism (Feynman and Hibbs 1965, Negele and Orland 1988); for a comprehensive review of Feynman's principle and Schwinger's dynamical principle in their historical setting see Yourgrau and Mandelstam (1968, Ch. 12). Hedin's work, however, is constructed within the canonical (i.e. Hamiltonian) formulation of quantum mechanics and thus differs from the path-integral description which is based on the Lagrangian formalism. An "on-the-mass-shell" approximation to the GWA ($\Sigma^{GW}(k;\varepsilon) \to \Sigma^{GW}(k;\varepsilon_k^0)$) is due to Quinn and Ferrell (1958). Pratt (1960) in his search for generalising the Hartree–Fock theory, has arrived at an eigenvalue problem which involves the screened exchange, i.e. GW, SE operator. Starting from an expression for the correlation energy due to Hubbard (1958), Phillips (1961) has also arrived at the screened-exchange, GW, approximation.

9.2. *Details of the GW approximation exposed (Part I)*

For Σ^{GW} in terms of the *exact* G and W (see Sec. 9) we have

$$\begin{aligned}\Sigma^{GW}(\mathbf{r}t,\mathbf{r}'t') &= \frac{i}{\hbar}G(\mathbf{r}t,\mathbf{r}'t')W(\mathbf{r}t^+,\mathbf{r}'t'),\\ \Sigma^{GW}(\mathbf{r},\mathbf{r}';\varepsilon) &= \frac{i}{\hbar}\int_{-\infty}^{\infty}\frac{d\varepsilon'}{2\pi\hbar}G(\mathbf{r},\mathbf{r}';\varepsilon-\varepsilon')W(\mathbf{r},\mathbf{r}';\varepsilon')e^{-i\varepsilon'\eta/\hbar}, \quad (\eta\downarrow 0).\end{aligned} \tag{174}$$

The + sign in the argument of W in the first expression, and thus the exponential function on the RHS of the second expression, has its root in the discontinuity of the GF at $t' = t$ (see Eq. (8); see also Appendix B) and the instantaneous part of $W(\mathbf{r}t,\mathbf{r}'t')$ (or the energy independent part of $W(\mathbf{r},\mathbf{r}';\varepsilon)$) that would otherwise render the above expressions ambiguous. We have $W(\mathbf{r}t,\mathbf{r}'t') = v_c(\mathbf{r}-\mathbf{r}')\delta(t-t') + \overline{W}(\mathbf{r}t,\mathbf{r}'t')$, and thus

$$W(\mathbf{r},\mathbf{r}';\varepsilon) = v_c(\mathbf{r}-\mathbf{r}') + \overline{W}(\mathbf{r},\mathbf{r}';\varepsilon). \tag{175}$$

Making use of Eqs. (94), (95) and (100) we have[91]

$$\overline{W}(\mathbf{r},\mathbf{r}';\varepsilon) = \sum_s w_s(\mathbf{r})w_s^*(\mathbf{r}')\left\{\frac{1}{\varepsilon - e_s + i\eta} - \frac{1}{\varepsilon + e_s - i\eta}\right\}, \quad \eta\downarrow 0, \tag{176}$$

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[91] For $|\varepsilon| \to \infty$, $\overline{W}(\varepsilon)$ diminishes like $1/\varepsilon^2$.

where

$$w_s(\mathbf{r}) := 2^{1/2} \int d^3r' v_c(\mathbf{r}-\mathbf{r}')\varrho_s(\mathbf{r}'); \tag{177}$$

thus $w_s(\mathbf{r})$ is the electrostatic potential due to the deviation of the charge distribution in an N-electron excited state with respect to that in the N-electron GS. With this expression and the Lehmann representation for $G(\varepsilon)$ in Eq. (11), using Cauchy's residue theorem (Titchmarsh 1939, p. 102) the ε'-integral in Eq. (174) is easily evaluated, leading to

$$\Sigma^{GW}(\mathbf{r},\mathbf{r}';\varepsilon) = \Sigma^{Gv_c}(\mathbf{r},\mathbf{r}') + \Sigma^{G\overline{W}}(\mathbf{r},\mathbf{r}';\varepsilon), \tag{178}$$

where

$$\begin{aligned}
\Sigma^{Gv_c}(\mathbf{r},\mathbf{r}') &:= \frac{-1}{\hbar} v_c(\mathbf{r}-\mathbf{r}') \sum_s \theta(\mu-\varepsilon_s) f_s(\mathbf{r}) f_s^*(\mathbf{r}') \\
&\equiv -\frac{1}{2\hbar} v_c(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r},\mathbf{r}'), \\
\Sigma^{G\overline{W}}(\mathbf{r},\mathbf{r}';\varepsilon) &:= \frac{1}{\hbar} \sum_{s,s'} f_s(\mathbf{r}) f_s^*(\mathbf{r}') w_{s'}(\mathbf{r}) w_{s'}^*(\mathbf{r}') \\
&\quad \times \left\{ \frac{\theta(\varepsilon_s-\mu)}{\varepsilon-\varepsilon_s-e_{s'}+i\eta} + \frac{\theta(\mu-\varepsilon_s)}{\varepsilon-\varepsilon_s+e_{s'}-i\eta} \right\}.
\end{aligned} \tag{179}$$

The static contribution Σ^{Gv_c} is exactly the Fock exchange self-energy Σ^F (see Subsecs. 4.6, 5.1 and 6.3 where we have $\Sigma^{HF}(\mathbf{r},\mathbf{r}') \equiv \hbar^{-1} v_H(\mathbf{r};[n])\delta(\mathbf{r}-\mathbf{r}') + \Sigma^F(\mathbf{r},\mathbf{r}')$). Since $e_{s'} \geq 0$ for *all* s', the first (second) term inside the braces on the RHS of Eq. (179) is finite, i.e. non-singular, for $\varepsilon < \mu\,(\varepsilon > \mu)$ — notice that the θ-function restricts the range of ε_s-values contributing to each term. Let now $\varepsilon_v(\varepsilon_c)$ correspond to the largest (smallest) ε_s below (above) μ (for our earlier reference to ε_v and ε_c see Subsec. 4.2). Let in addition

$$e_{\min} := \min\{e_{s'}\}\big|_{s'\neq 0}, \tag{180}$$

where we have excluded the *trivial* $e_{s=0}$.[92] It follows that the singularity — i.e. "branch point" for systems in the thermodynamic limit (see Subsecs. 2.1 and 2.2) — of $\Sigma^{GW}(\varepsilon)$ closest to μ from below is located at

$$\varepsilon_< := \varepsilon_v - e_{\min} \tag{181}$$

[92] From Eq. (101) we observe that $\varrho_{s=0}(\mathbf{r}) \equiv 0$ — for systems with non-degenerate GS, $e_{\min} > 0$.

and the one from above μ at

$$\varepsilon_> := \varepsilon_c + e_{\min} . \tag{182}$$

Compare $\varepsilon_<$ and $\varepsilon_>$ with μ_N and μ_{N+1} in Subsec. 4.2, respectively. It can explicitly be shown that for $\varepsilon \in (\varepsilon_<, \varepsilon_>)$, $\Sigma^{GW}(\varepsilon)$ *is* Hermitian. In case W has been evaluated within the RPA, making use of the *same* GF as has been employed in the calculation of Σ^{GW} (which may be a G_0), it holds (see Eq. (14) above and the text following it): $e_{\min} = (\varepsilon_c - \varepsilon_v)$. In such a case we have

$$\varepsilon_> - \varepsilon_< \equiv (\varepsilon_c - \varepsilon_v) + 2e_{\min} = 3(\varepsilon_c - \varepsilon_v) . \tag{183}$$

Hence, within the GWA, making use of a G_0 and the corresponding W^{RPA} (by which we mean the W obtained through approximating P by $P_0[G_0]$ in $W = v_c + v_c P W$ — see Eq. (92) and Subsec. 8.4), the *possible* QPs whose energies may turn out to lie inside the interval $(\varepsilon_<, \varepsilon_>)$ possess infinite lifetimes. In view of the above (see in particular the text *directly* following Eq. (179)) it follows that

$$\widetilde{\Sigma}^{G\overline{W}}(\mathbf{r}, \mathbf{r}'; z) := \frac{1}{\hbar} \sum_{s,s'} f_s(\mathbf{r}) f_s^*(\mathbf{r}') w_{s'}(\mathbf{r}) w_{s'}^*(\mathbf{r}') \times \left\{ \frac{\theta(\varepsilon_s - \mu)}{z - \varepsilon_s - e_{s'}} + \frac{\theta(\mu - \varepsilon_s)}{z - \varepsilon_s + e_{s'}} \right\} \tag{184}$$

is the analytic continuation of $\Sigma^{G\overline{W}}(\varepsilon)$ into the complex z-plane: we have indeed

$$\Sigma^{G\overline{W}}(\varepsilon) = \lim_{\eta \downarrow 0} \widetilde{\Sigma}^{G\overline{W}}(\varepsilon \pm i\eta) \quad \text{for } \varepsilon \gtrless \mu ; \tag{185}$$

when $\varepsilon \in (\varepsilon_<, \varepsilon_>)$, η can be put identically to zero. It can explicitly be shown that similar to the exact $\widetilde{\Sigma}(z)$, $\widetilde{\Sigma}^{GW}(z)$ satisfies the relation (*c.f.* Eq. (40))

$$\widetilde{\Sigma}^{GW}(z^*) = \widetilde{\Sigma}^{GW^\dagger}(z) . \tag{186}$$

By explicit calculation, the relations in Eq. (51) can be shown to be satisfied by $\widetilde{\Sigma}^{GW}(z)$ *provided* that for the $\widetilde{G}(z)$ in Eq. (51) use is made of the expression in Eq. (27), i.e. of the *same* expression that we have employed in determining $\Sigma^{GW}(\varepsilon)$ in Eq. (174) and thus $\widetilde{\Sigma}^{G\overline{W}}(z)$ in Eq. (184).

Through rearranging the terms in the above expressions, Σ^{GW} can be written in the alternative form

$$\Sigma^{GW}(\varepsilon) = \Sigma_{SX}(\varepsilon) + \Sigma_{CH}(\varepsilon)\,, \tag{187}$$

where

$$\Sigma_{SX}(\mathbf{r},\mathbf{r}';\varepsilon) := \frac{-1}{\hbar}\sum_{s}\theta(\mu-\varepsilon_s)\{v_c(\mathbf{r}-\mathbf{r}')+\overline{W}(\mathbf{r},\mathbf{r}';\varepsilon-\varepsilon_s)\}f_s(\mathbf{r})f_s^*(\mathbf{r}')\,,$$

$$\Sigma_{CH}(\mathbf{r},\mathbf{r}';\varepsilon) := \frac{1}{\hbar}\sum_{s,s'}\frac{f_s(\mathbf{r})f_s^*(\mathbf{r}')w_{s'}(\mathbf{r})w_{s'}^*(\mathbf{r}')}{\varepsilon-\varepsilon_s-e_{s'}+i\eta}\,. \tag{188}$$

Here Σ_{SX} denotes the so-called "screened-exchange" and Σ_{CH} the "Coulomb-hole" part of Σ^{GW}; the former is clearly a generalisation of the Fock exchange SE in which the v_c is corrected for by the dynamic screening function $\overline{W}$ (see Σ^{Gv_c} in Eq. (179)) and the latter represents the influence of the Coulomb repulsion in creating or shaping the region around *each* electron that is deficient of other electrons (this region corresponds thus to a "hole") — recall that within the (unscreened) Hartree–Fock scheme, there is no Coulomb repulsion between electrons of *opposite* spin. It is sometimes mentioned that Σ_{SX} is the contribution of the residues of the integrand on the RHS of Eq. (174) at the poles of $G(\varepsilon - \varepsilon')$ (which as can be observed from the first expression in Eq. (188) is indeed the case), and that, by analogy, Σ_{CH} were the contribution of the residues of the same integrand at the poles of $\overline{W}(\varepsilon')$. The latter assertion is *incorrect*. The reason for this lies in the ambiguity associated with the equality of the magnitude of the imaginary parts of the poles in the Lehmann (-type) representations for $G(\varepsilon)$ and $\overline{W}(\varepsilon)$ (in both representations this is equal to η); with equal imaginary parts, the functions $G(\varepsilon - e_{s'} + i\eta)$ and $\overline{W}(\varepsilon-\varepsilon_s-i\eta)$, which are encountered upon a straightforward application of the residue theorem, are indefinite. This ambiguity is removed by taking the imaginary part associated with the poles in the Lehmann (-type) representations for $G(\varepsilon)$ and $\overline{W}(\varepsilon)$ to be $i\eta$ and $i\eta'$, respectively. The expressions in Eq. (188) follow from the assumption that $\eta' > \eta$ (*following* the derivation, η' is set equal to η). One obtains an equally correct result by assuming $\eta' < \eta$, but by doing so the resulting Σ_{SX} will not involve the *physical* $\overline{W}$, but $\widetilde{\overline{W}}(\varepsilon - \varepsilon_s - i\eta)$ which for $\varepsilon - \varepsilon_s > 0$ coincides with the limit of $\widetilde{\overline{W}}(z)$ where z approaches the real energy axis from the side for which $\widetilde{\overline{W}}(z) \to \overline{W}^{\dagger}(\varepsilon - \varepsilon_s)$. Assumption $\eta' > \eta$, on the other hand, leads to the *"physical"* $\overline{W}(\varepsilon - \varepsilon_s)$ for all $(\varepsilon - \varepsilon_s)$; it leads to the *"unphysical"* $\widetilde{G}(\varepsilon - e_{s'} + i\eta')$ for $\varepsilon - e_{s'} < \mu$, however.

9.3. *Some sum-rules concerning* $\Sigma^{G\overline{W}}$

Consider

$$\widetilde{\Sigma}^{G\overline{W}\prime\prime}(z) := \frac{1}{2i}\{\widetilde{\Sigma}^{G\overline{W}}(z) - \widetilde{\Sigma}^{G\overline{W}\dagger}(z)\}\,. \tag{189}$$

From the analyses following Eq. (179) — that for $\varepsilon < \mu$, $\theta(\varepsilon_s - \mu)\delta(\varepsilon - \varepsilon_s - e_{s'}) = 0$, and for $\varepsilon > \mu$, $\theta(\mu - \varepsilon_s)\delta(\varepsilon - \varepsilon_s + e_{s'}) = 0$ —, the following sum rules are readily obtained (we make use of Eqs. (185) and (186))

$$\frac{1}{\pi}\int_{-\infty}^{\mu} d\varepsilon \Sigma^{G\overline{W}\prime\prime}(\mathbf{r},\mathbf{r}';\varepsilon) = \frac{1}{2\hbar}\rho(\mathbf{r},\mathbf{r}')\mathcal{W}_1(\mathbf{r},\mathbf{r}')\,, \tag{190}$$

$$\frac{-1}{\pi}\int_{\mu}^{+\infty} d\varepsilon \Sigma^{G\overline{W}\prime\prime}(\mathbf{r},\mathbf{r}';\varepsilon) = \frac{1}{\hbar}\left(\delta(\mathbf{r}-\mathbf{r}') - \frac{1}{2}\rho(\mathbf{r},\mathbf{r}')\right)\mathcal{W}_1(\mathbf{r},\mathbf{r}')\,, \tag{191}$$

$$\frac{1}{\pi}\int_{-\infty}^{\mu} d\varepsilon\,\varepsilon \Sigma^{G\overline{W}\prime\prime}(\mathbf{r},\mathbf{r}';\varepsilon) = \frac{1}{\hbar}\left\{\Xi_<(\mathbf{r},\mathbf{r}')\mathcal{W}_1(\mathbf{r},\mathbf{r}') - \frac{1}{2}\rho(\mathbf{r},\mathbf{r}')\mathcal{W}_2(\mathbf{r},\mathbf{r}')\right\}\,, \tag{192}$$

$$\begin{aligned}\frac{-1}{\pi}\int_{\mu}^{+\infty} d\varepsilon\,\varepsilon \Sigma^{G\overline{W}\prime\prime}(\mathbf{r},\mathbf{r}';\varepsilon) = \frac{1}{\hbar}\Bigg\{&\Xi_>(\mathbf{r},\mathbf{r}')\mathcal{W}_1(\mathbf{r},\mathbf{r}') \\ &+ \left(\delta(\mathbf{r}-\mathbf{r}') - \frac{1}{2}\rho(\mathbf{r},\mathbf{r}')\right)\mathcal{W}_2(\mathbf{r},\mathbf{r}')\Bigg\}\,,\end{aligned} \tag{193}$$

where[93]

$$\mathcal{W}_1(\mathbf{r},\mathbf{r}') := \sum_{s'} w_{s'}(\mathbf{r})w_{s'}^*(\mathbf{r}')\,, \tag{194}$$

$$\mathcal{W}_2(\mathbf{r},\mathbf{r}') := \sum_{s'} e_{s'}w_{s'}(\mathbf{r})w_{s'}^*(\mathbf{r}')\,. \tag{195}$$

For $\Xi_<(\mathbf{r},\mathbf{r}')$ and $\Xi_>(\mathbf{r},\mathbf{r}')$ see Eqs. (17) and (18).

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[93] Note that $\mathcal{W}_2(\mathbf{r},\mathbf{r}') \equiv \frac{1}{2}\overline{W}_{\infty 2}(\mathbf{r},\mathbf{r}') := \frac{1}{2}\lim_{|\varepsilon|\to\infty} \varepsilon^2\overline{W}(\mathbf{r},\mathbf{r}';\varepsilon)$.

Making use of Eqs. (177) and (152) we obtain

$$\sum_{s'} w_{s'}(\mathbf{r}) w_{s'}^{*}(\mathbf{r}') \equiv \int d^3 r_1 d^3 r_2\, v_c(\mathbf{r} - \mathbf{r}_1)$$
$$\times \left[\frac{-1}{\pi} \int_0^{\infty} d\varepsilon \chi''(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \right] v_c(\mathbf{r}_2 - \mathbf{r}') \,, \qquad (196)$$

where the term inside the square brackets is closely related to the pair-correlation function $g(\mathbf{r}_1, \mathbf{r}_2)$ and the GS electronic density (see Eqs. (152) and (157); see also Eq. (154)). We have further

$$\sum_{s'} e_{s'} w_{s'}(\mathbf{r}) w_{s'}^{*}(\mathbf{r}') \equiv \frac{1}{2} \int d^3 r_1 d^3 r_2\, v_c(\mathbf{r} - \mathbf{r}_1)$$
$$\times \left[\frac{-2}{\pi} \int_0^{\infty} d\varepsilon \varepsilon\, \chi''(\mathbf{r}_1, \mathbf{r}_2; \varepsilon) \right] v_c(\mathbf{r}_2 - \mathbf{r}') \,. \qquad (197)$$

The term within the square brackets is $\chi_{\infty_2}(\mathbf{r}_1, \mathbf{r}_2)$ as defined in Eqs. (118), (122) and (153). This is interesting in view of the fact that (i) when the external potential is local (i.e. $w \equiv 0$), the χ_0 corresponding to the "non-interacting" KS system with the exact but *local* v_{xc} has the property that $\chi_{0;\infty_2} \equiv \chi_{\infty_2}$ — see Subsecs. 8.5 and 8.10; (ii) for cases where $w \not\equiv 0$, it is in principle possible to construct a "non-interacting" KS Hamiltonian whose ensemble χ_0 yields the *exact* $\rho(\mathbf{r}, \mathbf{r}')$; the v_{xc} corresponding to this Hamiltonian is explicitly non-local — in Subsec. 9.7 we shall briefly touch upon the pertinent formalism.

9.4. *Details of the GW approximation exposed (Part II)*

In calculations of Σ^{GW} in terms of some G_0, one can with advantage exploit the fact that the spectral representation of G_0 is fully determined in terms of the eigenvalues and eigenfunctions of a "non-interacting" Hamiltonian, H_0, which is both independent of ε and Hermitian. This does not apply to $\overline{W}^{(0)}[G_0]$; even within the RPA, the polarisation function is both ε dependent and, in general, non-Hermitian.[94] A further practical difficulty concerning evaluation of $\overline{W}$ is associated with the required inversion of $\epsilon(\varepsilon)$ in Eq. (94). Hence, unless one relies upon some plasmon-pole-type of approximation for $\overline{W}$ (see Subsecs. 8.9

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[94] Here $\overline{W}^{(0)}[G_0]$ is defined in analogy with $P^{(0)}[G_0]$ in Subsec. 8.4; see also Subsec. 7.6.

and 8.10), *practical* considerations imply the necessity that Σ^{GW} be expressed in an alternative form, one that does not involve the spectral representation of $\overline{W}(\varepsilon)$ (as in Eq. (188)) *and* avoids integration of $\overline{W}(\varepsilon')$ along the real ε'-axis (as in Eq. (174)); in the thermodynamic limit, for real ε' calculation of $\overline{W}(\varepsilon')$ requires evaluation of integrals that involve singular integrands, accurate determination of which is extremely time-consuming; moreover, along the ε'-axis, $\overline{W}(\varepsilon')$ has fine and sharp structures, necessitating evaluation of this function over a fine mesh of ε'-points which is also computationally a demanding task. For these reasons, as we shall clarify below, the following alternative expression for Σ_{CH} is superior to, e.g., that in Eq. (188):

$$\Sigma_{CH}(\mathbf{r},\mathbf{r}';\varepsilon) = \frac{1}{\hbar}\sum_{s} f_s(\mathbf{r})f_s^*(\mathbf{r}')$$
$$\times \left\{ \theta(\varepsilon-\varepsilon_s)\overline{W}(\mathbf{r},\mathbf{r}';\varepsilon-\varepsilon_s) - \int_{-i\infty}^{+i\infty}\frac{d\varepsilon'}{2\pi i}\frac{\widetilde{\overline{W}}(\mathbf{r},\mathbf{r}';\varepsilon')}{\varepsilon-\varepsilon'-\varepsilon_s}\right\}. \tag{198}$$

This expression is obtained from that for Σ^{GW} in Eq. (174) through deformation of the contour of the ε'-integration, corresponding to $\Sigma^{G\overline{W}}$ in Eq. (179), from along the *real* ε'-axis to one along the *imaginary* ε'-axis (Quinn and Ferrell 1958, Godby, Schlüter and Sham 1986, 1988, Farid, Daling, Lenstra and van Haeringen 1988). In doing so, appropriate account has been taken of the "poles" of both $\widetilde{G}(z)$ and $\widetilde{\overline{W}}(z)$ — see work by Farid, Daling, Lenstra and van Haeringen (1988) for details. For $\varepsilon = \varepsilon_s$, the integrand of the integral on the RHS of Eq. (198) has a singularity at $\varepsilon' = 0$. It can be shown that this singularity can be made harmless by considering the ε'-integral as a Cauchy principal-value integral,[95] and simultaneously defining $\theta(0) = 1/2$.

Consider the integral

$$\int_{-i\infty}^{+i\infty}\frac{d\varepsilon'}{2\pi i}\frac{\widetilde{\overline{W}}(\varepsilon')}{z-\varepsilon'} =: \widetilde{\Upsilon}(z), \tag{199}$$

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[95] The principal-value integral according to *Cauchy* is defined by the requirement that singular point(s) of the pertinent integrand be positioned in the *middle* of the infinitesimal interval(s) over which integration is excluded.

which occurs on the RHS of Eq. (198), with $z = \varepsilon - \varepsilon_s$. It can be shown that $\widetilde{\Upsilon}(z)$ is analytic everywhere on the complex z-plane where $\widetilde{\overline{W}}(z)$ is analytic (Titchmarsh 1939, p. 99),[96] except that it has a continuous branch cut along the imaginary axis. Moreover, from the Plemelj relations (Davies 1985, pp. 313–321 and 340, Noble 1958, pp. 141–147) it follows that we have (below $\varepsilon_s^{\pm} := \varepsilon_s \pm \eta$, with $\eta \downarrow 0$)

$$\widetilde{\Upsilon}(\varepsilon_s^{+} - \varepsilon_s + iy) - \widetilde{\Upsilon}(\varepsilon_s^{-} - \varepsilon_s + iy) = \widetilde{\overline{W}}(iy)\,, \quad y \text{ real}. \tag{200}$$

Thus on changing ε from below ε_s to above ε_s, the two terms inside the braces on the RHS of Eq. (198) exactly cancel each other's discontinuity. Using the uniqueness of analytic continuation (Titchmarsh 1939, pp. 139 and 140), it follows that $\widetilde{\Sigma}_{CH}(z)$ is analytic across the lines $\mathrm{Re}(z) = \varepsilon_s$, for *all* s. This is in accordance with Eq. (188) where we have only to do with $+i\eta$ and *not* with a combination of both $+i\eta$ and $-i\eta$.

From all the expressions for $\Sigma^{GW}(\varepsilon)$ given above, it can explicitly be shown that $\Sigma^{GW''}(\varepsilon = \mu) = 0$ (*c.f.* Eq. (78)) where $\Sigma^{GW''}(\varepsilon)$ is defined in Eq. (189); from Σ_{SX} and Σ_{CH} as given in Eqs. (188) and (198), respectively, it can directly be observed that for $\varepsilon = \mu$ the terms involving $\overline{W}(\mathbf{r}, \mathbf{r}'; \varepsilon - \varepsilon_s)$ *exactly* cancel. For ε deviating from μ, $\overline{W}(\mathbf{r}, \mathbf{r}'; \varepsilon - \varepsilon_s)$ is seen to contribute to $\Sigma^{GW}(\varepsilon)$ for that set of ε_s's for which $[\theta(\mu - \varepsilon_s) - \theta(\varepsilon - \varepsilon_s)]$ is non-vanishing; this defines a window of "relevant" ε_s values in the interval $[\mu, \varepsilon]$, for the case $\mu < \varepsilon$, and $[\varepsilon, \mu]$, for the case $\varepsilon < \mu$. Thus as far as the contribution of $\overline{W}(\mathbf{r}, \mathbf{r}'; \varepsilon - \varepsilon_s)$ to $\Sigma^{GW}(\varepsilon)$ is concerned, it is only necessary to know $\overline{W}(\varepsilon')$ for $\varepsilon' \in [0, |\mu - \varepsilon|]$ (recall that $\overline{W}(-\varepsilon') \equiv \overline{W}(\varepsilon')$). Therefore, the expression in Eq. (198) indeed amounts to a substantial computational simplification in particular in cases where one needs to know $\Sigma^{GW}(\varepsilon)$ for a small range of ε values close to μ.

Finally, as can be directly seen from the explicit expression for $\Sigma^{G\overline{W}}(\varepsilon)$, determination of the asymptotic behaviour of $\Sigma^{G\overline{W}''}(\varepsilon)$ for $\varepsilon \to \mu$ is far from trivial, since this requires an *a priori* knowledge of not only $\{\varepsilon_s\}$ but also $\{e_s\}$ close to μ (see our remarks in Subsec. 6.4).

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[96] Strictly, for this to be true two conditions have to be satisfied: (i) The Hölder condition (Davies 1985, pp. 313–321 and 340, Noble 1958, pp. 11–13), $|\widetilde{\overline{W}}(\varepsilon') - \widetilde{\overline{W}}(\varepsilon'')| < A|\varepsilon' - \varepsilon''|^{\alpha}$ with $A > 0$, $\alpha > 0$; (ii) The asymptotic relation $\widetilde{\overline{W}}(\varepsilon') \sim' \varepsilon'^{-\beta}$ for $|\varepsilon'| \to \infty$, with $\beta > 0$. Analyticity of $\widetilde{\overline{W}}(\varepsilon')$ along the imaginary axis implies that the Hölder condition is automatically satisfied. We know also that $\beta = 2$.

9.5. *Some approximation schemes within the GW approximation*

Complete neglect of $\Sigma^{G\overline{W}}$ on the RHS of Eq. (178) amounts to one of the possible approximations within the *GW*A scheme. In this way one recovers the Fock exchange SE of the conventional Hartree–Fock method.

A more sophisticated approximation is the so-called COHSEX, *COulomb Hole with Screened EXchange* (Hedin 1965). This is obtained through suppression of the energy dependence of $\overline{W}$ (or $\widetilde{\overline{W}}$) in the expressions for Σ_{SX} and Σ_{CH} (see Eqs. (178), (188) and (197)). By doing so, Σ_{XC} transforms into a *form* similar to Σ^{Gv_c} (see Eq. (179)), with v_c however replaced by $v_c + \overline{W}(\varepsilon = 0) \equiv W(\varepsilon = 0)$. In other words, in this scheme Σ_{SX} reduces to the Fock-exchange SE in terms of the *static* screened Coulomb interaction function. As for the "Coulomb-hole" part of the SE, as presented in Eqs. (188) and (198),[97] it can be easily shown that within this approximation $\Sigma_{CH}(\mathbf{r},\mathbf{r}';\varepsilon) \to (1/[2\hbar])\overline{W}(\mathbf{r},\mathbf{r}';0)\sum_s f_s(\mathbf{r})f_s^*(\mathbf{r}')$. Making use of the completeness of the Lehmann amplitudes (Eq. (15)), one arrives at

$$\Sigma^{COHSEX}(\mathbf{r},\mathbf{r}') = -\frac{1}{2\hbar}W(\mathbf{r},\mathbf{r}';0)\rho(\mathbf{r},\mathbf{r}') + \frac{1}{2\hbar}\overline{W}(\mathbf{r},\mathbf{r};0)\delta(\mathbf{r}-\mathbf{r}')\,. \tag{201}$$

The second term on the RHS of Eq. (201) has an interesting physical interpretation (Hedin 1965). Consider two point charges held fixed at $\mathbf{r}$ and $\mathbf{r}'$. If there were no screening, then the potential energy of the point charge at $\mathbf{r}$ due to that at $\mathbf{r}'$ amounted to $v_c(\mathbf{r}-\mathbf{r}')$.[98] Because of the polarisation effects, in reality this energy amounts to $W(\mathbf{r},\mathbf{r}';0)$. The difference between the two energies, i.e. $\overline{W}(\mathbf{r},\mathbf{r}';0)$ (see Eq. (175)), is thus the *induced* potential energy. The force $\mathbf{F}$ on the point charge at $\mathbf{r}$ associated with the latter potential energy is equal to $-\nabla\overline{W}(\mathbf{r},\mathbf{r}';0)$. By taking the limit $\mathbf{r}' \to \mathbf{r}$, one obtains the force $\mathbf{F}$ on the point charge at $\mathbf{r}$ brougbt about by its own presence, through polarising its surrounding; $\mathbf{F} := -\lim_{\mathbf{r}'\to\mathbf{r}} \nabla\overline{W}(\mathbf{r},\mathbf{r}';0)$. Because of the symmetry property (see Eqs. (175), (176) and (106)) $\overline{W}(\mathbf{r},\mathbf{r}';\varepsilon) = \overline{W}(\mathbf{r}',\mathbf{r};\varepsilon)$, for this self-induced force $\mathbf{F} = -\nabla\{\frac{1}{2}\overline{W}(\mathbf{r},\mathbf{r};0)\}$ holds. Thus we observe that the contribution of Σ_{CH} to Σ^{GW} within the COHSEX approximation describes the self-induced static force exerted on a point charge introduced into the system (compare the

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[97] For $\varepsilon = \varepsilon_s$, the RHS of Eq. (188) involves $\sum_{s'} w_{s'}w_{s'}^\dagger/(-e_{s'})$, which from Eq. (176) is seen to be equal to $\frac{1}{2}\overline{W}(0)$. Alternatively, in Eq. (198) we have $\overline{W}(0)\int_{-i\infty}^{+i\infty} d\varepsilon'/(2\pi i[\varepsilon-\varepsilon'-\varepsilon_s]) = \frac{1}{2}\mathrm{sgn}(\varepsilon-\varepsilon_s)\overline{W}(0)$. Using $[\theta(\varepsilon-\varepsilon_s) - \frac{1}{2}\mathrm{sgn}(\varepsilon-\varepsilon_s)] = \frac{1}{2}$, we again obtain $\frac{1}{2}\overline{W}(0)$.

[98] Note the e^2 in the definition for v_c.

term enclosed by the curly braces in the expression for $\mathbf{F}$ with the second term on the RHS of Eq. (201)).

Evaluation of the ε'-integral along the imaginary energy axis on the RHS of Eq. (198) is not, from the practical point of view, a difficult task: here one has to do with a very smooth integrand which, moreover, decreases like $\sim' \varepsilon'^{-3}$ for large values of $|\varepsilon'|$. Thus one might consider to retain the dependence on ε' of $\widetilde{\overline{W}}(\varepsilon')$ in the integral along the imaginary energy axis, but replace $\overline{W}(\varepsilon - \varepsilon_s)$ in the expressions for Σ_{SX} (Eq. (188)) and Σ_{CH} (Eq. (198)) by its *static* counterpart; in doing so, the $\theta(\varepsilon - \varepsilon_s)$ which pre-multiplies this $\overline{W}(0)$ in Eq. (198) must be retained (see text immediately following Eq. (200) above). This approximation which has been introduced by Toet (1987), is referred to as the *Static-Pole Approximation* (SPA). From the discussions in Subsec. 9.4 (in the paragraph following Eq. (200)), it is clear that knowledge of $\overline{W}(\varepsilon')$ for ε' within the interval $[0, |\mu - \varepsilon|]$ suffices to calculate the contribution due to $\overline{W}(\varepsilon - \varepsilon_s)$ to $\Sigma^{GW}(\varepsilon)$. From the fact that for small values of $|\varepsilon'|$, $\overline{W}(\varepsilon') = \overline{W}(0) + o(1)$, it follows that for sufficiently small values of $|\mu - \varepsilon|$, indeed $\overline{W}(\varepsilon - \varepsilon_s)$ to a very good approximation can be replaced by $\overline{W}(0)$.

9.6. *Large-$|\varepsilon|$ behaviour of $\Sigma^{GW}(\varepsilon)$*

In Subsec. 8.3 we studied in some detail the large-$|\varepsilon|$ behaviour of $\chi(\varepsilon)$, $P(\varepsilon)$ and some related functions (operators). The explicit expression for $\Sigma^{GW}(\varepsilon)$ as presented in Eq. (179) gives us the opportunity also to expose some of the interesting features of $\Sigma^{GW}(\varepsilon)$ for $|\varepsilon| \to \infty$. Here we consider three leading asymptotic terms of $\Sigma^{GW}(\varepsilon)$,

$$\Sigma^{GW}(\varepsilon) \sim \Sigma^{Gv_c} + \frac{\Sigma^{GW}_{\infty_1}}{\varepsilon} + \frac{\Sigma^{GW}_{\infty_2}}{\varepsilon^2}\,, \quad \text{for} \quad |\varepsilon| \to \infty\,, \tag{202}$$

where $\Sigma^{GW}_{\infty_1}$ and $\Sigma^{GW}_{\infty_2}$ are independent of ε. Making use of Eqs. (15), (194), (195) and some simple algebra one obtains

$$\Sigma^{GW}_{\infty_1}(\mathbf{r}, \mathbf{r}') = \frac{1}{\hbar}\delta(\mathbf{r} - \mathbf{r}')\mathcal{W}_1(\mathbf{r}, \mathbf{r}')\,, \tag{203}$$

$$\Sigma^{GW}_{\infty_2}(\mathbf{r}, \mathbf{r}') = G_{\infty_2}(\mathbf{r}, \mathbf{r}') - \frac{1}{\hbar}\{\rho(\mathbf{r}, \mathbf{r}') - \delta(\mathbf{r} - \mathbf{r}')\}\mathcal{W}_2(\mathbf{r}, \mathbf{r}')\,. \tag{204}$$

Note that according to Eq. (31), $-\hbar\{\rho(\mathbf{r}, \mathbf{r}') - \delta(\mathbf{r} - \mathbf{r}')\}$ is equal to the zeroth energy moment of $A_p(\mathbf{r}, \mathbf{r}'; \varepsilon)$. From Eq. (203) we observe that $\Sigma^{GW}_{\infty_1}$ is fully determined by the zeroth energy moment of $\chi''(\varepsilon)$ — see Eqs. (194) and (196).

As is evident, $\Sigma^{GW}_{\infty_2}$ is partly determined by G_{∞_2}. This, according to Eq. (35), is in turn fully governed by n and ρ. The remaining contributions to $\Sigma^{GW}_{\infty_2}$ are due to ρ and $\mathcal{W}_2$. The latter, according to Eqs. (195), (197) and (153), is determined by χ_{∞_2} which following Eqs. (122) and (153) is, again, seen to be fully controlled by n and ρ.

In view of the occurrence of G_{∞_2} in the asymptotic expansion of $\Sigma^{GW}(\varepsilon)$ for $|\varepsilon| \to \infty$, it is interesting to consider $G_{0;\infty_2}$. For this the following is easily obtained

$$G_{0;\infty_2}(\mathbf{r},\mathbf{r}') = \hbar\Bigg\{ \left[\frac{-\hbar^2}{2m_e}\nabla^2 + v(\mathbf{r}) + v_H(\mathbf{r};[n_0]) + v_L(\mathbf{r})\right]\delta(\mathbf{r}-\mathbf{r}') \\ + w(\mathbf{r},\mathbf{r}') + v_{NL}(\mathbf{r},\mathbf{r}')\Bigg\}, \qquad (205)$$

where v_L and v_{NL} are, respectively, the local and non-local potentials that we have assumed to be, in addition to the Hartree potential, incorporated in the "non-interacting" Hamiltonian to which G_0 corresponds. The density n_0 in the argument of v_H, denotes the density in the GS of $\widehat{H}_0$. We have to point out that $G_{0;\infty_2}$ in Eq. (205) is distinct from that in Eq. (36) which corresponds to the truly non-interacting system of electrons. Since the "non-interacting" Hamiltonian $\widehat{H}_0$ in the present case incorporates $v_H + v_L + v_{NL}$, the corresponding Dyson equation reads $G = G_0 + G_0\Sigma_1 G$, with Σ_1 defined in Eq. (98). Thus, according to the first equality in Eq. (43) we have $\Sigma_{1;\infty_0} = \hbar^{-2}\{-G_{0;\infty_2} + G_{\infty_2}\}$. From Eqs. (35), (205), (98) and (99) we therefore obtain $\Sigma^{GW}_{\infty_0} \equiv (\Sigma_{1;\infty_0} + \hbar^{-1}[v_H + v_L + v_{NL}]) - \hbar^{-1}v_H \equiv \Sigma^{Gv_c}$, which is indeed the leading-order term on the RHS of Eq. (202).

9.7. *The DFT revisited: An explicitly non-local effective potential*

Since the last term on the RHS of Eq. (35) is *non-local*, the $G_{0;\infty_2}$ corresponding to the *commonly-used* KS Hamiltonian *cannot* possibly be exactly identical to G_{∞_2}, although in this case v_H is exactly reproduced (see text following Eq. (99)). However, within the framework the DFT which is designed to yield the exact $n(\mathbf{r})$ — thus assuming $w(\mathbf{r},\mathbf{r}') \equiv 0$ —, the effective potential v_{eff} in the KS equation (Eq. (135)) can take on different forms depending on how the energy functional $F[n]$ in Eq. (107) is decomposed. The *multiplicative*, or, *explicitly local* form that this potential apparently has in Eq. (135) is a consequence of the following decomposition

$$F[n] = T_s[n] + E_H[n] + E_{xc}[n]\,, \tag{206}$$

where

$$T_s[n] := 2\int d^3r \sum_i \theta(\mu - \varepsilon_i)\psi_i^*(\mathbf{r})\left[\frac{-\hbar^2}{2m_e}\nabla^2\right]\psi_i(\mathbf{r})\,, \tag{207}$$

$$E_H[n] := \frac{1}{2}\int d^3r d^3r' v_c(\mathbf{r}-\mathbf{r}')n(\mathbf{r})n(\mathbf{r}')\,; \tag{208}$$

the orbitals $\{\psi_i(\mathbf{r})\}$ in Eq. (207) are the eigenfunctions of the KS Hamiltonian in Eq. (135) above. Equation (206) *defines* $E_{xc}[n]$ as the difference between $F[n]$ and $T_s[n] + E_H[n]$. It follows that $v_{\text{eff}}(\mathbf{r};[n]) := v(\mathbf{r}) + \delta\{E_H[n] + E_{xc}[n]\}/\delta n(\mathbf{r}) \equiv v(\mathbf{r}) + v_H(\mathbf{r};[n]) + v_{xc}(\mathbf{r};[n])$ is *explicitly* local. If now, following Kohn and Sham (1965), $F[n]$ is decomposed like

$$F[n] = T_s[n] + E_H[n] + E_x[n] + E_c[n]\,, \tag{209}$$

with $T_s[n]$ and $E_H[n]$ defined as in Eqs. (207) and (208), respectively, and

$$E_x[n] := \frac{-1}{2}\int d^3r d^3r' v_c(\mathbf{r}-\mathbf{r}')\rho_0(\mathbf{r},\mathbf{r}')\rho_0(\mathbf{r}',\mathbf{r})\,, \tag{210}$$

where (see Eq. (135))

$$\rho_0(\mathbf{r},\mathbf{r}') := 2\sum_i \theta(\mu - \varepsilon_i)\psi_i(\mathbf{r})\psi_i^*(\mathbf{r}')\,, \tag{211}$$

from the Euler–Lagrange equation for $E_v[n]$ the following KS (1965) equation is obtained:

$$\left[\frac{-\hbar^2}{2m_e}\nabla^2 + v(\mathbf{r}) + v_H(\mathbf{r};[n]) + \mathsf{v}_c(\mathbf{r};[n])\right]\psi_i(\mathbf{r}) \\ -\frac{1}{2}\int d^3r' v_c(\mathbf{r}-\mathbf{r}')\rho_0(\mathbf{r},\mathbf{r}')\psi_i(\mathbf{r}') = \varepsilon_i\psi_i(\mathbf{r})\,, \tag{212}$$

which is "Hartree–Fock like", rather than "Hartree like" (*c.f.* Eq. (135)). The correlation energy functional $E_c[n]$ is *defined* through Eq. (209) and its corresponding potential

$$\mathsf{v}_c(\mathbf{r};[n]) := \frac{\delta E_c[n]}{\delta n(\mathbf{r})} \tag{213}$$

is referred to at the "correlation potential". Above we have denoted the single-particle reduced density matrix corresponding to the KS equation (Eq. (212)), i.e. the Dirac-Fock reduced density matrix, by $\rho_0(\mathbf{r}, \mathbf{r}')$, to indicate that this is *not* identical to the exact one-particle density matrix, although $\rho_0(\mathbf{r}, \mathbf{r}) \equiv n(\mathbf{r})$, the *exact* GS electron density. The reason for this lies in the fact that in arriving at Eq. (212), only variations in $n(\mathbf{r})$ around the GS charge density have been considered; for obtaining a KS equation (see Footnote 78) whose eigenfunctions yield the exact $\rho(\mathbf{r}, \mathbf{r}')$ through $\sum_i \lambda_i \psi_i(\mathbf{r}) \psi_i^*(\mathbf{r}')$, it is necessary that variations of ρ around the ρ corresponding to the GS are considered (Gilbert 1975; see also Donnelly and Parr (1978) and Valone (1980)), in which case the pertinent KS equation will aquire an *explicitly non-local* correlation potential.[99] Nevertheless, it is interesting to note that through choosing H_0 to coincide with the *explicitly* non-local KS Hamiltonian in Eq. (212), in addition to preserving the important property $n_0(\mathbf{r}) \equiv n(\mathbf{r})$, it is ensured that the corresponding $G_{0;\infty_2}$ incorporates a non-local term involving v_c. However, there are two differences between this $G_{0;\infty_2}$ and G_{∞_2}: (i) the expression for $G_{0;\infty_2}$ involves $\mathsf{v}_c(\mathbf{r};[n])$, which does *not* feature in the expression for G_{∞_2}; (ii) the one-particle reduced density matrix in $G_{0;\infty_2}$ is $\rho_0(\mathbf{r}, \mathbf{r}')$ whereas that in Eq. (35) is $\rho(\mathbf{r}, \mathbf{r}')$.

In view of the above considerations, it is instructive to consider the following expression for the GS total energy due to Galitskii and Migdal (1958)[100]

$$E_{N,0} = -i \int d^3r \lim_{\mathbf{r}' \to \mathbf{r}} \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi\hbar} e^{i\varepsilon\eta/\hbar} \times \left\{ \left[\varepsilon - \frac{\hbar^2}{2m_e} \nabla^2 + v(\mathbf{r}) \right] G(\mathbf{r}, \mathbf{r}'; \varepsilon) + \int d^3r'' w(\mathbf{r}, \mathbf{r}'') G(\mathbf{r}'', \mathbf{r}'; \varepsilon) \right\} , \tag{214}$$

where we have suppressed the energy due to the inter-ionic (or background) interaction; in addition, we have multiplied the RHS of this equation by 2 in

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[99] That $\rho_0 \not\equiv \rho$, is easiest shown by pointing out that unlike ρ, ρ_0 *is* idempotent: $\int d^3r'' \rho_0(\mathbf{r}, \mathbf{r}'') \rho_0(\mathbf{r}'', \mathbf{r}') = \rho_0(\mathbf{r}, \mathbf{r}')$, whereas $\int d^3r'' \rho(\mathbf{r}, \mathbf{r}'') \rho(\mathbf{r}'', \mathbf{r}') < \rho(\mathbf{r}, \mathbf{r}')$. See, e.g., the work by Dreizler and Gross (1990, p. 47). The non-idem-potency of $\rho(\mathbf{r}, \mathbf{r}')$ manifests itself in the deviation of λ_i from either zero or unity. This implies that the density-functional framework for constructing the exact ρ is an *ensemble* formalism, to be contrasted with a *pure-state* formalism.

[100] For some technical details concerning application of this expression see the paper by Farid, Godby and Needs (1991).

order to account for the trace over the spin of the electrons. An aspect of substantial practical interest is that the total energy is determined by the zeroth- and first-order ε-moments of $G(\varepsilon)$. In the present work we have attempted to expose the intimate connections that exist between the energy moments and the large-$|\varepsilon|$ behaviour of various correlation functions on the one hand, and the relationship between these and the GS charge density and the single-particle reduced density matrix on the other. Equation (214) provides yet another evidence for this. Through making use of (below $\eta \downarrow 0$) — see Eqs. (16), (17) and (26) —

$$-i\int_{-\infty}^{+\infty} \frac{d\varepsilon}{2\pi\hbar}\, e^{i\varepsilon\eta/\hbar} G(\mathbf{r},\mathbf{r}';\varepsilon) = -iG(\mathbf{r}t,\mathbf{r}'t^{+}) \equiv \frac{1}{2}\rho(\mathbf{r},\mathbf{r}')\,, \tag{215}$$

$$-i\int_{-\infty}^{+\infty} \frac{d\varepsilon}{2\pi\hbar}\, e^{i\varepsilon\eta/\hbar} \varepsilon G(\mathbf{r},\mathbf{r}';\varepsilon) = \sum_{s} \theta(\mu-\varepsilon_s)\varepsilon_s f_s(\mathbf{r}) f_s^{*}(\mathbf{r}') \equiv \Xi_{<}(\mathbf{r},\mathbf{r}')\,, \tag{216}$$

while employing both the exact and the approximate expression on the RHS of Eq. (22), it can readily be verified that[101]

$$\begin{aligned} E_{N,0} = {} & \int d^3r v(\mathbf{r}) n(\mathbf{r}) + \int d^3r d^3r' w(\mathbf{r},\mathbf{r}') \rho(\mathbf{r},\mathbf{r}') \\ & + \int d^3r \lim_{\mathbf{r}'\to\mathbf{r}} \left[\frac{-\hbar^2}{2m_e}\nabla^2\right] \rho(\mathbf{r},\mathbf{r}') \\ & + \frac{N(N-1)}{2} \int d^3r d^3r' v_c(\mathbf{r}-\mathbf{r}') g(\mathbf{r},\mathbf{r}')\,, \end{aligned} \tag{217}$$

$$\begin{aligned} & \frac{N(N-1)}{2} \int d^3r d^3r' v_c(\mathbf{r}-\mathbf{r}') g(\mathbf{r},\mathbf{r}') \\ & \qquad \approx \frac{1}{2} \int d^3r d^3r' v_c(\mathbf{r}-\mathbf{r}') n(\mathbf{r}) n(\mathbf{r}') \equiv E_H[n]\,. \end{aligned} \tag{218}$$

From the considerations in Subsec. 8.8 we know, that for systems without off-diagonal long-range order (i.e., involving no superfluidity or superconductivity), for $\|\mathbf{r}-\mathbf{r}'\| \to \infty$ we have $N(N-1)g(\mathbf{r},\mathbf{r}') \to n(\mathbf{r})n(\mathbf{r}')$, so that the

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[101] For a similar expression see the books by March, Young and Sampanthar (1967, p. 10), and Dreizler and Gross (1990, Appendix A).

(Hartree) approximation in Eq. (218) is seen to correspond to neglect of the short-range correlation effects.

Our above considerations demonstrate that calculation of Σ^{GW} in terms of G_0 and W_0 ($\equiv W^{RPA}[G_{KS}]$ — see text following Eq. (183)) corresponding to the KS "non-interacting" Hamiltonian, whose ground-state $n(\mathbf{r})$ is identical to that of the fully interacting system, incorporates such correlation effects that are very specific to $\Sigma^{GW}[G]$, i.e. the Σ^{GW} as evaluated in terms of the *exact* G and W.

9.8. *Self-consistent calculations*

Consider the following *unconstrained* self-consistent procedure for the calculation of G (or Σ): Start with a given "non-interacting" Hamiltonian H_0 which in addition to v_H contains $v_L + v_{NL}$. Calculate $\Sigma^{GW}[G_0]$, i.e. Σ^{GW} in terms of the GF pertaining to H_0 (see Subsecs. 7.6 and 9). Through solution of the Dyson equation calculate $G_{\{i=1\}}$, with $G_{\{i+1\}} = (I - G_0\Sigma_{\mathrm{I}}^{GW}[G_{\{i\}}])^{-1}G_0$, where (see Subsec. 7.6) $\Sigma_{\mathrm{I}}^{GW}[G_{\{i\}}] := \Sigma^{GW}[G_{\{i\}}] - \hbar^{-1}(v_L + v_{NL})$, with $G_{\{i\}}$ the GF corresponding to the ith iteration, $i = 0, 1, \ldots, M_{sc}$ ($G_{\{0\}} \equiv G_0$). Here M_{sc} is the number of iterations beyond which the changes in the matrix elements of, say, $G_{\{i\}}$ are negligible. In practice, it may happen that this straightforward process of iteration does not converge (a known fact concerning iterative solution of non-linear equations), in which case one has to employ a more refined scheme. A strategy that is not sophisticated and in other contexts has proved to be useful (Kerker 1981, Dederichs and Zeller 1983 — for completeness, see the paper by Ho, Ihm and Joannopoulos (1982)), consists in calculating $G_{\{i+1\}}$, for $i \geq 1$, in terms of $\Sigma_{\mathrm{I}}^{GW}[(1-\alpha)G_{\{i-1\}} + \alpha G_{\{i\}}]$ with $\alpha \in (0, 1]$ (for small values of i, $\alpha \ll 1$) rather than $\Sigma_{\mathrm{I}}^{GW}[G_{\{i\}}]$. We note that for the linear combination $(1-\alpha)G_{\{i-1\}} + \alpha G_{\{i\}}$ to be meaningful, it is necessary that the values of μ corresponding to $G_{\{i-1\}}$ and $G_{\{i\}}$ are identified before the two functions are linearly combined.

It should be evident that there is no *a priori* reason for considering the converged G, as obtained according to the above strategy, in any sense superior to the non-self-consistent G, i.e. $G_{\{1\}}$. The following two points should clarify this statement. First, the non-linearity of the problem at hand implies existence of a multiplicity of solutions for G, so that "the" self-consistent G may be entirely different from that which one has set out to calculate (see Sec. 7). We have to emphasise that even though there is no compelling argument in favour of $G_{\{1\}}$, one may argue that if G_0 has been a "good" zeroth-order approximation to G, the contribution of Σ_1^{GW} to G should amount to a "minor" correction, in which case $G_{\{1\}}$ appropriately takes this correction into account. Second, disregarding the first point, in order to assess the accuracy, or even qualitative correctness, of the self-consistent G, one needs to know the significance of those contributions in $(\Sigma - \hbar^{-1}v_H)$ that have been neglected in Σ^{GW}: a G that is self-consistent within an approximate framework, is *not* necessarily "closer" to the exact G than a non-self-consistent G.

From the above we conclude that for performing reliable self-consistent calculations, one has to define some appropriate *norm* (which can be different depending on the nature of the questions being addressed) which imposes constraints on the self-consistent solution. These constraints can be either so-called "equality constraints" or "inequality constraints", or some combination of both. To the former class of constraints belongs the requirement that the GS charge densities corresponding to the non-interacting and interacting systems be *equal* (see Subsubsecs. 7.4.1 and 8.6.1), and to the latter that the GS total energy of the self-consistent G be minimal (see Subsec. 9.7). We shall now argue that a self-consistent calculation must involve at least one "inequality constraint". Obviously, since the functional form of Σ^{GW} is fixed, it follows that for satisfying the "equality constraints" it is necessary that H_0 be adjusted, through variations in $(v_L + v_{NL})$ — in this way G_0 is varied and thus also $\Sigma^{GW}[G_0]$. Therefore within an "equality-constraint" scheme one adjusts the non-interacting Hamiltonian, with respect to which perturbation expansion is carried out, until the required equality is satisfied (by, say, $G_{\{i\}}$, where i may take on the value 1 if for whatever reason $G_{\{1\}}$ is preferred above $G_{\{M_{sc}\}}$). Such constraint *cannot* in itself guarantee even the qualitative correctness of the self-consistent solution. This follows from the obvious fact that the quantities on both sides of an "equality constraint" are to be calculated in parallel, so that at self-consistency one may be satisfying an incorrect equality. Thus one comes to realise that the self-consistent G must, for instance, yield the lowest GS total energy (in so far as possible within the GWA) for it to be at least qualitatively correct.

In applying the above strategy for the self-consistent calculation of G, it is important that the "equality constraints" are mutually compatible and that they can indeed be enforced. Here the known theorems of the DFT can be of substantial value. For instance, if for a given system one can assume that its GS electronic distribution $n(\mathbf{r})$ is non-interacting v-representable (see Footnote 7), one can immediately draw the significant conclusion that the mapping between $v_L(\mathbf{r})$ and $n(\mathbf{r})$ is *invertible* (Hohenberg and Kohn 1964). This implies that (i) it is possible to impose the "equality constraint" that the GS charge density of the non-interacting system be identical to that of the interacting system; (ii) that v_L is uniquely determined (up to a trivial additive constant). We recall the very important role played by the GS charge density and the reduced one-particle density matrix in determining the large-ε behaviour of various correlation functions as well as the values for the ε-moment integrals corresponding to the "imaginary" parts (i.e., the branch-cut discontinuities) of these functions (see Subsecs. 4.6, 8.3, 8.8, 8.9, 9.3 and 9.6).

As for the compatibility of the constraints, the freedom in adjusting v_{NL} suggests that in principle it should be possible that, for self-consistency also some say, *static* two-point correlation function pertaining to the non-interacting system be made to coincide with that of the interacting system. However, since the *local* part of v_{NL} has been absorbed in v_L, this requirement may not be compatible with the one that is to be enforced by v_L. We point out that even the requirement that both $n_0(\mathbf{r})$ and $\rho_0(\mathbf{r}, \mathbf{r}')$ corresponding to the non-interacting system be identical to those corresponding to the interacting system *cannot* be met, despite the fact that $n(\mathbf{r}) = \rho(\mathbf{r}, \mathbf{r})$. This is due to the non-idempotency of ρ (see Footnote 99) that rules out the possibility of describing ρ in terms of a pure state; for imposing the condition $\rho_0 \equiv \rho$, an ensemble formalism for the many-body perturbation theory must be adopted. Nevertheless, one can attempt to find an optimal v_{NL} such that the corresponding ρ_0 resembles ρ as closely as possible (according to some well-specified norm). This constitutes an "ineqnality constraint".

It is interesting to note that since $\Sigma^{GW}(\varepsilon)$, similar to the *exact* $\Sigma(\varepsilon)$, is Hermitian at $\varepsilon = \mu$ (see Subsec. 6.4 and 9.4) — of course the μ corresponding to Σ^{GW} is different from the exact μ, corresponding to Σ —, it is possible to impose the "equality constraint" that at $\varepsilon = \mu$, $\Sigma^{GW}(\varepsilon)$ and $\hbar^{-1}(v_L + v_{NL})$ be identical (see Eq. (98)). Such a constraint, provided accompanied by an appropriate "inequality constraint", should give rise to a non-interacting Hamiltonian that at energies close to μ describes the behaviour of the QPs relatively accurately.

All self-consistent methods (such as those described above) are rendered impracticable (except for relatively simple systems) by the fact that at various stages of calculation, a number of integrations have to be carried out. If these integrals are not evaluated with sufficient accuracy, it is most likely that the consequent errors will eventually dominate the outcomes which have to be obtained over in principle many self-consistency cycles. The present author (Farid 1997a, b) has proposed a way out of this problem and the computational results indicate the proposed approach to be extremely reliable.

9.9. *Some technical aspects*

Here we briefly discuss a number of aspects that are of practical relevance. Since most of the calculations in the past have concerned periodic crystals, and it is natural that this will remain an active area of research in future, here we shall focus on some aspects specific to evaluation of Σ^{GW} for these systems in three spatial dimensions (for notational conventions see Appendix A). We explicitly consider Σ^{GW} as evaluated in terms of a G_0, i.e. $\Sigma^{GW}[G_0]$.

Let $\{\mathcal{R}_i|\mathbf{R}_j\}$ denote an element of the *space group* of the Hamiltonian of the system, both interacting and non-interacting. For a two-point function $F(\mathbf{r},\mathbf{r}';\varepsilon)$ pertaining to the system, which may be $\Sigma^{GW}(\mathbf{r},\mathbf{r}';\varepsilon)$, $G(\mathbf{r},\mathbf{r}';\varepsilon)$, $\chi(\mathbf{r},\mathbf{r}';\varepsilon)$, etc., we have

$$\{\mathcal{R}_i|\mathbf{R}_j\}F(\mathbf{r},\mathbf{r}';\varepsilon) := F(\boldsymbol{\beta}_i\mathbf{r} + \boldsymbol{\tau}_i + \mathbf{R}_j, \boldsymbol{\beta}_i\mathbf{r}' + \boldsymbol{\tau}_i + \mathbf{R}_j;\varepsilon) \equiv F(\mathbf{r},\mathbf{r}';\varepsilon)\,. \tag{219}$$

Here $\boldsymbol{\beta}_i$ stands for the *point-group* operation associated with $\{\mathcal{R}_i|\mathbf{R}_j\}$ and $\boldsymbol{\tau}_i$ for the corresponding *non-primitive* translation vector (which may be vanishing); $\mathbf{R}_j$ denotes a *primitive translation vector* (Slater 1965, Cornwell 1984). It can easily be shown that invariance of $F(\mathbf{r},\mathbf{r}';\varepsilon)$ under $\{\mathcal{R}_i|\mathbf{R}_j\}$ leads to the following result

$$F_{\mathbf{G},\mathbf{G}'}(\boldsymbol{\beta}_i\mathbf{k} + \mathbf{K}_i;\varepsilon) = e^{i[\boldsymbol{\beta}_i^{-1}(\mathbf{G}-\mathbf{G}')]\cdot\boldsymbol{\tau}_i} F_{\boldsymbol{\beta}_i^{-1}(\mathbf{G}+\mathbf{K}_i),\boldsymbol{\beta}_i^{-1}(\mathbf{G}+\mathbf{K}_i)}(\mathbf{k};\varepsilon)\,, \tag{220}$$

where $\boldsymbol{\beta}_i^{-1}$ denotes the inverse of $\boldsymbol{\beta}_i$ and $\mathbf{K}_i$ stands for the RLV that guarantees $\boldsymbol{\beta}_i\mathbf{k} + \mathbf{K}_i =: \mathbf{k}'_i$ to lie inside the 1BZ (we assume $\mathbf{k} \in$ 1BZ — $\mathbf{K}_i$ is generally vanishing except *possibly* for cases where $\mathbf{k}$ is on the boundary of the 1BZ). This result is of practical interest, as through it $F_{\mathbf{G},\mathbf{G}'}(\mathbf{k}'_i;\varepsilon)$, for all $\mathbf{k}'_i$'s that are distinct from $\mathbf{k}$, is obtained from an element of the set $\{F_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\varepsilon)\}$ by means of a mere phase-factor multiplication.

For our following discussions we take the expression for $\Sigma^{GW}(\varepsilon)$ as presented in Eqs. (188) and (198). We have

$$\Sigma^{GW}_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\varepsilon) = \frac{-1}{\hbar\Omega} \sum_{\mathbf{k}'\in 1\mathrm{BZ}} \sum_{\mathbf{K},\mathbf{K}'} z_{\mathbf{K},\mathbf{K}'}(\mathbf{G},\mathbf{G}';\mathbf{k},\mathbf{k}';\varepsilon)\,, \tag{221}$$

where

$$
\begin{aligned}
&\mathcal{Z}_{\mathbf{K},\mathbf{K}'}(\mathbf{G},\mathbf{G}';\mathbf{k},\mathbf{k}';\varepsilon) \\
&:= \sum_{\ell} d_{\ell,\mathbf{k}-\mathbf{k}'}(\mathbf{K}) d^{*}_{\ell,\mathbf{k}-\mathbf{k}'}(\mathbf{K}') \Big\{ \theta(\mu - \varepsilon_{\ell}(\mathbf{k}-\mathbf{k}')) v_{c;\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}') \\
&\quad + [\theta(\mu - \varepsilon_{\ell}(\mathbf{k}-\mathbf{k}')) - \theta(\varepsilon - \varepsilon_{\ell}(\mathbf{k}-\mathbf{k}))] \overline{W}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon - \varepsilon_{\ell}(\mathbf{k}-\mathbf{k}')) \\
&\quad + \int_{-i\infty}^{+i\infty} \frac{d\varepsilon'}{2\pi i} \frac{\widetilde{\overline{W}}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon')}{\varepsilon - \varepsilon' - \varepsilon_{\ell}(\mathbf{k}-\mathbf{k}')} \Big\}, \qquad (222)
\end{aligned}
$$

with

$$
v_{c;\mathbf{G},\mathbf{G}'}(\mathbf{k}) := \frac{e^2/\epsilon_0}{\|\mathbf{k}+\mathbf{G}\|^2}\, \delta_{\mathbf{G},\mathbf{G}'} \qquad (223)
$$

the $(\mathbf{G},\mathbf{G}')$-matrix element of the Coulomb interaction function in the wave-vector representation; $\{d_{\ell;\mathbf{k}}(\mathbf{K})\}_{\mathbf{K}}$ denotes the set of Fourier coefficients corresponding to the periodic part of a Bloch-type eigenfunction of H_0, normalised according to $\sum_{\mathbf{K}} d_{\ell;\mathbf{k}}(\mathbf{K}) d^{*}_{\ell;\mathbf{k}}(\mathbf{K}) = 1$; ℓ denotes the band index and $\mathbf{k} \in$ 1BZ. The $\mathbf{k}$-summation over the 1BZ is replace by a $\mathbf{k}$-integration according to $\sum_{\mathbf{k}\in 1\mathrm{BZ}} (\ldots) \to (\Omega/[2\pi]^3) \int_{1\mathrm{BZ}} d^3k\, (\ldots)$, with Ω the volume of the crystal. When appropriate (see further on), this integration is subsequently replaced by a *finite* summation. The most commonly-used summation method is one based on the so-called *special-points* technique (Baldereschi 1973, Chadi and Cohen 1973, Monkhorst and Pack 1976). For any *lattice structure*, the theory underlying this technique prescribes a well-specified set of (finite) sampling points within the 1BZ over which the integrand is to be averaged, with each sampling being weighed by a well-specified symmetry-related weight factor. There are a number of different procedures for generating these points, each of which gives rise to different sets of "special points" and the associated sets of weight factors. We shall not go into the details of these methods, however there is one crucial aspect concerning "special points" to which we should like draw attention:

All "special-points" methods deal with evaluation of integrals of the form $\int_{\mathbf{k}\in 1\mathrm{BZ}} d^3k\, \mathcal{B}(\mathbf{k}) =: \mathcal{I}$, where $\mathcal{B}(\mathbf{k})$ is assumed to be periodic over the entire reciprocal space, repeating the form it has over the 1BZ, *and* to have the complete *lattice* point-group symmetry. A typical example for $\mathcal{B}(\mathbf{k})$ is the band energy $\varepsilon_{\ell}(\mathbf{k})$. Consequently, $\mathcal{B}(\mathbf{k})$ can be expanded into a symmetrised discrete Fourier series. The constant term in this series is the sought-after $\mathcal{I}$. The special-points sampling methods employ such sets of sampling points that *up to a certain order* render the combined contribution of all harmonics of $\mathcal{B}(\mathbf{k})$ vanishing. Since with a finite number of sampling points, it is not possible to inactivate *all* harmonics of $\mathcal{B}(\mathbf{k})$, the sufficiency of a finite set of special points in a particular application depends on the magnitudes of the spectral coefficients in the mentioned symmetrised Fourier series that have not been addressed by the adopted set of "special points". Now as for the *crucial* point to which we have referred above, for certain functions, $\mathcal{B}(\mathbf{k})$, *though smooth over the 1BZ*, the assumption of *periodicity* over the entire reciprocal space may imply discontinuous behaviour in their extended form, or in the derivatives of this, at the zone boundaries. It follows that these functions possess large spectral contents associated with high orders of their Fourier coefficients.[102] This leads to slow convergence, with respect to the number of the sampling points, towards the exact $\mathcal{I}$. It is important to bear this point in mind, for sometimes authors seek to justify their use of a special-points-sampling strategy through arguments that merely show the "smoothness" of the involved integrands *over* the 1BZ and not that of their periodic extensions. We should emphasise that use of discrete sampling methods for evaluation of the BZ integrals is *not* a fundamental necessity, rather a practical one: many of the present-day calculations concerning realistic models of solids would not be practicable if the necessary BZ integrals had to be evaluated by means of such methods as the linear or quadratic "tetrahedron" methods (Lehmann and Taut 1972, Rath and Freeman 1975, Methfessel, Boon and Muller 1983,1987), which are based upon subdivision of the 1BZ into small tetrahedra, inside each of which the BZ-integral is evaluated analytically following a linear (Lehmann and Taut 1972, Rath and Freeman 1975) or quadratic (Methfessel, Boon and Muller 1983,1987) expansion of some part (mostly the denominator) of the integrand.

The expression for $\Sigma^{GW}_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\varepsilon)$ in Eqs. (221) and (212) brings out a number of points which are worth mentioning.

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[102] Consider the function $k^2/2$ over $[-\pi/a_c, \pi/a_c)$, the 1BZ of a one-dimensional periodic system. Although admittedly very "smooth" in the usual sense of the word, when periodically extended over the entire k-axis, $k^2/2$ at $k = \pm\pi/a_c$ has a derivative discontinuity, in magnitude equal to $2\pi/a_c$. The component with index m of the Fourier expansion of the periodically-extended $k^2/2$ for large m decreases like $1/m^2$, implying a very slow convergence of the BZ integral of $k^2/2$ according to a "special-points" technique (for a convergence of, say, 1%, it is required that $m \simeq 10$ — in three dimensions, this amounts to requiring $\simeq 10^3$ sampling points over the 1BZ). In contrast, a Gaussian-quadrature method yields the exact value for this BZ-integral upon the second sampling and beyond.

First, as indicated above, the BZ-integration in Eq. (221) is most likely to be evaluated by means of one or another type of averaging technique over a *discrete* set of $\mathbf{k}'$-points. In view of this, the following should be taken into consideration:

(i) As is apparent from Eq. (223), the Coulomb interaction matrix element $v_{c;\mathbf{G},\mathbf{G}}(\mathbf{k})$ is singular at $\mathbf{k}+\mathbf{G}=\mathbf{0}$ (for $\mathbf{k}$ in the *interior* of the 1BZ, this equation is satisfied only when $\mathbf{G}=\mathbf{0}$). Consequently, the integrand of the $\mathbf{k}'$-integration has to be regularised prior to applying any discrete summation technique; the BZ-integral corresponding to the singular part (which in the process of regularisation has been taken apart) has to be evaluated by means of some appropriate method — for instance a sampling approach in the spherical polar coordinate system, with the origin being centred at the singular point of the integrand. In view of our above remarks concerning limitations of the "special-points" method, it is advantageous for the convergence rate of the BZ-integral in Eq. (221), as function of the number of the "special points", that the "regularised" $v_{c;\mathbf{G},\mathbf{G}}(\mathbf{k})$ be free from discontinuities or sharp "edges".

(ii) The screening potential $\overline{W}$ is short-ranged *only* in metallic systems (see Footnote 48); for semiconducting or insulating systems, the screening is *not* complete and therefore $\overline{W}$, like v_c, is singular (see however Subsubsec. 7.4.1 and Footnote 64). Moreover, the behaviour of $\overline{W}_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\varepsilon)$ close to its singularity (i.e., for $\mathbf{k}\to\mathbf{0}$ — see further on, however) is in general anisotropic, i.e. it depends on the direction of $\mathbf{k}$ along which $\mathbf{k}\to\mathbf{0}$, cubic crystals being exceptional in this respect; see works by Falk (1960), Pick, Cohen and Martin (1970), Baldereschi and Tosatti (1978, 1979) and Baldereschi, Car and Tosatti (1979). To analyse the behaviour of $\overline{W}_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\varepsilon)$, it is necessary to examine that of the matrix elements of the polarisation operator $P(\varepsilon)$. With

$$P_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\varepsilon)=\Pi_0(\mathbf{G},\mathbf{G}';\varepsilon)+\boldsymbol{\Pi}_1(\mathbf{G},\mathbf{G}';\varepsilon)\cdot\mathbf{k}$$
$$+\mathbf{k}\cdot\underline{\underline{\boldsymbol{\Pi}}}_2(\mathbf{G},\mathbf{G}';\varepsilon)\cdot\mathbf{k}+\mathcal{O}(\|\mathbf{k}\|^3)\,, \tag{224}$$

for $\mathbf{k}$ close to $\mathbf{0}$, the following relations can be shown to hold

$$\Pi_0(\mathbf{0},\mathbf{0};\varepsilon)=0\,;\quad \boldsymbol{\Pi}_1(\mathbf{0},\mathbf{0};\varepsilon)=\mathbf{0}\,; \tag{225}$$

$$\Pi_0(\mathbf{G},\mathbf{0};\varepsilon)=0\,;\quad \Pi_0(\mathbf{0},\mathbf{G}';\varepsilon)=0\,. \tag{226}$$

That is, the "head" element of $P(\mathbf{k};\varepsilon)$ (i.e. that corresponding to $\mathbf{G}=\mathbf{G}'=\mathbf{0}$) and "wing" elements (i.e. those corresponding to either $\mathbf{G}=\mathbf{0}$, $\mathbf{G}'\neq\mathbf{0}$ *or*

$\mathbf{G} \neq \mathbf{0}$, $\mathbf{G}' = \mathbf{0}$) are vanishing for $\mathbf{k} \to \mathbf{0}$, the former *quadratically* and the latter *linearly* in $\|\mathbf{k}\|$. In general, the tensor $\underline{\underline{\Pi}}_2$ has a full Cartesian matrix representation. For cubic crystals, however, it is, in this representation, a multiple of the unit matrix. From these results, taking into account the singular behaviour of $v_{c;\mathbf{G},\mathbf{G}}(\mathbf{k})$ for $\mathbf{k} + \mathbf{G} \to \mathbf{0}$, and application of the Sherman-Morrison-Woodbury formulae (Press, Teukolsky, Vettering and Flannery 1996, pp. 65–70) for inversion of matrices by partitioning (Pick, Cohen and Martin 1970), one arrives at the conclusion that the "head" element of $\overline{W}(\mathbf{k};\varepsilon)$ has a $1/\|\mathbf{k}\|^2$ type of singularity, the "wing" elements diverge like $1/\|\mathbf{k}\|$, and the "body" elements are regular. Again, except for cubic crystals, the divergence in the pertinent matrix elements of $\overline{W}(\mathbf{k};\varepsilon)$ is non-isotropic. We should emphasise that distinction has to be made between $\mathbf{k} \to \mathbf{0}$ and $\mathbf{k} = \mathbf{0}$ (Baldereschi and Tosatti 1978, 1979 — for some comments on this subject see the paper by Farid, Heine, Engel and Robertson (1993), Sec. IV). In our case, the point $\mathbf{k} = \mathbf{0}$, in combination with either $\mathbf{G} = \mathbf{0}$ or $\mathbf{G}' = \mathbf{0}$ (or both) has *no* significance: the matrix elements $\overline{W}_{\mathbf{G},\mathbf{0}}(\mathbf{k} = \mathbf{0};\varepsilon)$ and $\overline{W}_{\mathbf{0},\mathbf{G}'}(\mathbf{k} = \mathbf{0};\varepsilon)$ are vanishing, since an infinite periodic system cannot respond to a spatially constant perturbation without violating the charge conservation (see Footnote 80).[103] For some technical details see works by Gygi and Baldereschi (1986), von der Linden and Horsch (1988, Appendix C to this work) and Hott (1991).

(iii) In metals, the function $\theta(\mu - \varepsilon_\ell(\mathbf{k} - \mathbf{k}'))$ in Eq. (222) necessitates accurate knowledge of the Fermi surface in the $\mathbf{k}'$-space. It should be realised that also $\overline{W}$ in Eq. (222) is dependent on the geometry of the Fermi surface (see, e.g., P_0 in Subsec 8.5). Therefore, except for the simple metals, for which one may anticipate nearly spherical Fermi surfaces, accurate evaluation of $\Sigma^{GW}(\varepsilon)$ is computationally extremely demanding.

9.10. *A survey of computational works within the GW approximation*

Hedin (1965) has applied the GWA to calculate a variety of properties pertaining to the uniform-electron system. In particular he has calculated a number of parameters of the Landau Fermi-liquid theory. Rice (1965) at the same time as Hedin, starting from an expression due to Hubbard (1958) for the correlation-energy in terms of the SE operator, has calculated a number of Fermi-liquid

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[103] Recall that by charge neutrality, $v_{c;\mathbf{G},\mathbf{G}}(\mathbf{k})$ must be set equal to a constant (conventionally zero), when $\mathbf{G} = \mathbf{0}$ and $\mathbf{k} = \mathbf{0}$.

parameters. In his treatment, Rice has further considered some *static* local-field function (accounting for the vertex correction) that is neglected within the *GW*A. This static contribution is the Hubbard local-field function that we have discussed in Subsubsec. 8.6.3 (see Footnote 79).

There have been subsequent applications of the *GW*A to the uniform-electron system by a number of authors. In some of these, the vertex function has been approximately taken into account. Applications of the *GW*A to uniform-electron system are by Hedin (1965) and Lundqvist (1967, 1968, 1969). The latter author has calculated such functions as the momentum distribution function and the spectral function. Lundqvist and Samathiyakanit (1969), using the Galitskii-Migdal expression, have calculated the GS total energies at a number of metallic densities. Petrillo and Sacchetti (1988) have studied some consequences of the static local-field function on the results based on the *GW*A. This has been also subject of studies by Mahan and Sernelius (1989) and Frota and Mahan (1992). The last two works have been in part motivated by some controversies that seem to exist concerning the experimental values for the QP bandwidths in alkali metals in comparison with those calculated within the framework of the *GW*A and within a framework in which the vertex function has been taken into account (in an approximate way) *only* in the calculation of the screened interaction function W and *not* in that of the SE operator. As we observe from Fig. 12, within the standard *GW*A the vertex function Γ is neglected both in the expression for the polarisation function (this amounts to the RPA for this function — see Subsec. 8.4) and in that for the SE operator. The discussions in Subsec. 6.7 indicate that by a partial incorporation of the vertex function in the polarisation function, and neglect of it in the SE operator, the results may become less reliable as a consequence of disrupting the balance between the errors that otherwise would cancel. The numerical studies made so far on this issue (Mahan and Sernelius 1989, Frota and Mahan 1992) rely on very simple approximations for the local-field function G. For instance, these are energy independent and, moreover, do not have the correct behaviour at large values of k (see Subsubsec. 8.6.3).

The review article by Hedin and Lundquist (1969) gives an in-depth survey of the theory underlying the *GW* formalism as well as of a variety of related and relevant material. In particular, it contains some details concerning the core-polarisation effects and ways of incorporating these in approaches that primarily focus on the interaction amongst the valence (as opposed to the core) electrons. To this date this article remains the major reference source on the subject. In the intervening time the following brief surveys on the GWA have appeared: von Barth and Hedin (1974), Hybertsen and Louie (1987b), Godby (1992), Mahan (1994), Hedin (1995), Louie (1996). In Chapter 7 of the book by Inkson (1984), the method is described, and in Chapter 9 of the book by Fulde (1995), the approach is presented and further some applications of it to real solids are discussed.

Brinkman and Goodman (1966) in calculating the energy bands for silicon have applied the GWA, using the further approximation to which we in Subsec. 9.5 have referred as the COHSEX (Hedin 1965). In addition, the authors neglect the non-diagonal elements of the screened-interaction function W. Thus Brinkman and Goodman conclude "The results are not an improvement over the Slater approximation." Kane (1971) in his work entitled "Need for a Nonlocal Correlation Potential in Silicon" arrived at the conclusion that a "local approximation to exchange and correlation is inadequate for silicon" and that "screened Hartree–Fock exchange may provide the non-locality required to overcome ... difficulties." In a subsequent work, Kane (1972) applied the GWA to Si, using the Penn (1962) model for the dielectric function in the calculation of W. Subsequently, Inkson (1973) and Bennett and Inkson (1977, 1978), Inkson and Bennett (1978) and Sterne and Inkson (1984) have employed Σ^{GW}, using simplifying approximations in order to study effects of exchange and correlation on the energy bands of semiconductors. Brener (1975) has applied the COHSEX for calculating energy bands of diamond. Guinea and Tejedor (1980) have calculated Σ^{GW} for a model of a semiconductor, taking into account the *dynamic* screened interaction function as determined according to a plasmon-pole model.

Perhaps the first contribution that gave rise to the intensified activities that have extended to this date, concerning application of the GWA to realistic models of crystals, is due to Strinati, Mattausch and Hanke (1982). Works by Wang and Pickett (1983) and Pickett and Wang (1984) based on the local approximation for Σ^{GW} due to Sham and Kohn (1966) (see Subsec. 5.2) has been important in bringing out a salient feature of the SE operator ("dynamical correlation — *explicit excitation-dependent correction*") that is relevant to a correct description of the QP energy bands in solids. The mentioned activity has gathered momentum ever since the work by Hybertsen and Louie (1985) has appeared. The following, which most likely is an incomplete list, serves to indicate the activities in this area over a period of more than ten years:

Lannoo, Schlüter and Sham (1985) (quasi one-dimensional model semiconductor); Hybertsen and Louie (1985) (QP energies in Si), (1986) (C, Si, Ge, $LiCl$); Godby, Schlüter and Sham (1986, 1987, 1988) (QP energies of Si, $GaAs$, $AlAs$); Gygi and Baldereschi (1986) ("COHSEX", Si); Northrup, Hybertsen and Louie (1987) (QP energies in Na and Li), (1989) (Li, Na and Al); Hybertsen and Louie (1987a) (surface states of As and $Ge(111)$); von der Linden and Horsch (1988) (QP energies in Ge and a generalised plasmon-pole model); Hybertsen and Louie (1988) (surface states; $Ge(111) : As$ and $Si(111) : As$); Farid, Daling, Lenstra and van Haeringen (1988); Surh, Northrup and Louie (1988) (QP bandwidth of K); Gygi and Baldereschi (1989) (a simplified model for Σ^{GW}; results obtained for Si, Ge, $GaAs$ and $AlAs$); Zhang, Hybertsen, Coben, Louie and Tománek (1989) (ultrathin $AaAs/AlAs(001)$ superlattices); Zhang, Tománek, Cohen, Louie and Hybertsen (1989) (work on semiconductors without inversion symmetry); Zhu, Zhang, Louie and Cohen (1989) (work on relaxed $GaAs(110)$ surface); Godby and Needs (1989) (pressure-induced metal-insulator transition in Si); Saito, Zhang, Louie and Cohen (1989) (small metal clusters, using a jellium-sphere background); Hamada, Hwang and Freeman (1990) (Si, using "full-potential linearised augmented-plane-wave, FLAPW, method"); Farid, Godby and Needs (1990) (work on the ground-state total energy, Si); Engel, Farid, Nex and March (1991) (quasi one-dimensional model semiconductor); Hott (1991) (C, Si, Ge, Ga, As and InP); Chacham, and Louie (1991) (solid Hydrogen at Mbar pressures); Zhu and Louie (1991) (QP band-structures of thirteen semiconductors and insulators: Si, $LiCl$, AlP, $AlAs$, $AlSb$, GaP, $GaAs$, $GaSb$, InP, $InAs$, $InSb$, $Al_{0.5}Ga_{0.5}As$, $In_{0.53}Ga_{0.47}As$); Aryasetiawan (1992) (work on Ni); Shirley, Zhu and Louie (1992) (effects of core polarisation on QP energies; Si, Ge, $AlAs$ and $GaAs$); Shirley and Louie (1993) (solid C_{60}); Charlesworth, Godby and Needs (1993) (band-gap narrowing at an $Al/GaAs(110)$ interface); Rohlfing, Krüger and Pollmann (1993) (work on, amongst others, SiC); Farid (1994) (self-consistent GWA); Palummo, Reining, Godby, Bertoni, and Börnsen (1994) (electronic structure of cubic GaN); Rubio and Cohen (1995) (work on $GaAs_{1-x}N_x$ and $AlAs_{1-x}N_x$ ordered alloys); Engel, Kwon and Martin (1995) (comparison of results based on the GWA and those by Monte-Carlo techniques in a two-dimensional crystal); Backes, Bobbert and van Haeringen (1995) (plasmon and QP band energies in $\beta - SiC$); Wenzien, Käckell, Bechstedt and Cappellini (1995) (QP bands in SiC polytypes); Verdozzi, Godby and Holloway (1995) (work on a Hubbard cluster); Rohlfing, Krüger and Pollmann (1995a)

(QP band-structure of CdS — prototype of a $II - VI$ semiconductor; the GW results turn out to be satisfactory only after including "the complete cationic N shell in the pseudopotential"); Rohlfing, Krüger and Pollmann (1995b) (QP band-structure of bulk Si and the $Si(001) - (2 \times 1)$ surface — making use of a Gaussian-orbital basis set); Aryasetiawan and Gunnarsson (1995) (work on NiO); Onida, Reining, Godby, Del Sole and Andreoni (1995) (Na_4, Sodium tetramer); Aryasetiawan and Karlsson (1996) (work on Gd and NiO); Farid (1997a) (self-consistent GWA); Massidda, Continenza, Posternak, and Baldereschi (1997) (work on NiO and $CaCuO_2$).

A main conclusion that may be drawn from the above contributions is that for obtaining reliable results for the QP energies, it is important that *both* the energy dependence *and* the non-locality of Σ^{GW} (that for $\mathbf{r} \neq \mathbf{r}'$, $\Sigma^{GW}(\mathbf{r}, \mathbf{r}'; \varepsilon) \not\equiv 0$) be taken into account. Moreover, in solids it is essential that the W employed in the evaluation of Σ^{GW} takes account of the Umklapp scattering events, also referred to as the "local-field" effect (Falk 1960, Adler 1962, Wiser 1963), a manifestation of the fact that in electron-electron scattering processes inside a periodic lattice, wave-vectors are conserved only up to a RLV. It is due to recognition of these three issues to which the GWA owes its present-day widespread applications.

9.11. *Simplified schemes and suggestions*

As the brief exposition in Subsec. 9.9 should have made evident, determination of the ground and excited-states properties of systems within the GWA is relatively demanding, in terms of both the necessary computation times and the required computing facilities. Hence, truly large-scale applications of the GWA will become possible when Σ^{GW} can be cast into a simplified form that preserves the physically essential aspects contained in Σ^{GW}. In this connection it is relevant to mention that in a number of cases, the SE *corrections* (according to the GWA) to the LDA direct band-gaps over the entire BZs of semiconductors and insulators have turned out to be nearly dispersion-less. This observation has given rise to the notion of "scissors operator". This has been applied, for instance, to calculate the linear and second-harmonic optical succeptibilities for the $III - V$ semiconductors AlP, $AlAs$, GaP and $GaAs$ from the LDA-based electronic-structure results (Levine and Allan 1991a,b). One of the first successful attempts in the direction of simplifying Σ^{GW} is due to Gygi and Baldereschi (1989).

Recently, Rojas, Godby and Needs (1995) have successfully employed a strategy called "real-space-imaginary-time approach", which, owing to the multiplicative structure of the expressions for both Σ^{GW} and P^{RPA} in the $\mathbf{r}t$-representation, with advantage makes use of the technique of multi-dimensional fast-Fourier transform (i.e., FFT), thus reducing the number of required arithmetic operations, and consequently computation time, by considerable amount.

Concerning the static dielectric matrix, from which W is determined (see Eqs. (94) and (95)), a model due to Levine and Louie (1982) has proved (Hybertsen and Louie 1988, Zhu and Louie 1991) to be very reliable. We recall that for construction of $W(\varepsilon)$ within a plasmon-pole approximation in cases where the external potential is local (i.e. $w \equiv 0$), it is sufficient to know the *static* dielectric matrix and the GS charge density (see Subsecs. 8.9 and 8.10).

In Subsecs. 8.9 and 8.10 we have discussed the so-called plasmon-pole model for the description of the ε-dependence of the density-density correlation function, and consequently of the dynamic screened interaction function $W(\varepsilon)$. In fact, almost all of the contributions cited in Susbec. 9.10 make use of one or another type of the plasmon-pole model. In the work by Engel, Farid, Nex and March (1991), all of these models have been brought under the unifying scheme of the continued-fraction expansion for the branch-cut discontinuity (i.e., the "imaginary" part) of the dynamic density-density correlation function (see Subsec. 8.9). In the theory of the continued-fraction expansion, moments (here energy moments) of the branch-cut discontinuities of functions play a vital role. In Subsec. 9.3 we have presented explicit expressions for the first two ε-moments of $\Sigma^{G\overline{W}''}(\varepsilon)$ ($\equiv \Sigma^{GW''}(\varepsilon)$) which can be used to construct models for describing the ε-dependence of $\Sigma^{GW}(\varepsilon)$.[104] Such attempt has been made with considerable success by Kajueter and Kotliar (1996) in calculating the spectral properties of some lattice models (the asymmetric Anderson

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[104] I should like to acknowledge and thank Dr G. E. Engel who around 1992 brought up to me the idea of constructing such models for $\Sigma^{GW}(\varepsilon)$. No details were worked out at this time, however. In the paper by Engel, Farid, Nex and March (1991), it has been shown that for all energy moments of $\Sigma^{G\overline{W}''}(\varepsilon)$ up to order m (including the zeroth-order moment) to be correct, it is necessary that *all* energy moments of $\overline{W}''(\varepsilon)$ up to order m (including the zeroth-order moment) be correct. Since the commonly-used plasmon-pole models *only* reproduce the exact *first* energy moment (i.e. the f-sum rule) for the density-density correlation function, in the work by Engel, *et al.* (1991) it has been concluded that therefore *none* of the energy moments of $\Sigma^{G\overline{W}''}(\varepsilon)$ calculated through use of these plasmon-pole models is in principle correct.

lattice model and the Hubbard model). In our opinion, there stands nothing in the way of applying this technique for evaluation of $\Sigma^{GW}(\varepsilon)$.

9.12. *General trends and vertex corrections*

A general conclusion from the works cited in Subsec. 9.10 is that the *quasi-particle* spectra as obtained within the *GW* scheme are in good to excellent agreement with experimental results. There have been a number of attempts aimed at estimating the relative significance of the contributions of the higher-order SE diagrams to the fundamental QP-gap energy in semiconductors and insulators. These have pointed to the relative insignificance of these contributions.

The earliest studies towards estimating the influence of the vertex function, neglected within the *GW*A, are by Minnhagen (1974) and Bennett (1978). The former deals with the uniform-electron system and the latter with nearly-free-electron systems. Bennett concludes that in these systems, contribution of the vertex function to the band gap should be small — approximately 65 meV in a model system whose parameters correspond to silicon. More recently, there have been several studies of the same kind, all qualitatively confirming Bennett's conclusion. Daling and van Haeringen (1989), Daling, Unger, Fulde and van Haeringen (1991), Bobbert and van Haeringen (1994) arrive at the conclusion that the contribution of the only second-order *skeleton* SE diagram (i.e. the first-order vertex correction, neglected within the *GW*A — Fig. 12(b)) to the direct band gap in *Si* is relatively small, estimated to be on the order of 3% of the experimental value.[105] Work by Del Sole, Reining and Godby (1994) corroborate the latter conclusion.

In (Farid 1994,[106] 1997a), the present author has shown that the conclusions arrived at by the above authors are not conclusive. For details see (Farid 1997a). Here we only briefly mention that in these works, the exact GF not being available, the authors should not have restricted their considerations to the set of *skeleton* SE diagrams. Further, since in these works the correction to the *GW* band gap of *Si* has been derived through application of a first-order PT — based on the one-particle orbitals of the "non-interacting" system

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[105] In the work by Daling, *et al.* (1991) the correction is found to be less than 0.1 eV and in that by Bobbert and van Haeringen (1994) the best estimate amounts to 0.12 eV.

[106] This work is cited as Ref. 6 in de Groot, Bobbert and van Haeringen (1995). Incidentally, de Groot *et al.* in their Table II have mistakenly attributed "0.04883" to the work by the present author; the appropriate value is "0.06544".

—, the authors should have demonstrated that contribution of the GW self-energy to the non-interacting orbitals were small. In fact the calculations reported in (Farid 1994, 1997a) indicate that in general this *cannot* be the case. In their work, using the same model as employed in (Farid 1994), de Groot, Bobbert and van Haeringen (1995) conclude that vertex correction should be important. We note in passing that due to the non-locality and energy dependence of the SE operator in the QP equation (Eq. (58) above), the plasmon-pole model employed by de Groot, Bobbert and van Haeringen (1995) is *not* appropriate. Therefore it still remains an open question why the GWA has been so remarkably successful in accurately reproducing the QP band-gap energies of the thus-far studied semiconductors and insulators.

Finally, we mention that the spectral function (according to the notation in the present work, $A_p(\varepsilon)$ — see Eqs. (30) and (67)) as evaluated within the GWA, fails to reproduce the satellite structure observed in the photo-emission spectra (see Hedin and Lundqvist 1969, Almbladh and Hedin 1983) of even such simple metals as Na and Al (Aryasetiawan, Hedin and Karlsson 1996); see also Aryasetiawan and Gunnarsson (1995), Aryasetiawan and Karlsson (1996) and references herein. Since the satellite structure in the spectral function is of crucial influence on the energy moments of this function, analyses of Subsecs. 9.3 and 9.6 demonstrate that unless the non-interacting Hamiltonian in terms of which Σ^{GW} is evaluated, is capable of accurately reproducing such quantities as the *exact* GS electron density $n(\mathbf{r})$ and the *exact* reduced single-particle density matrix $\rho(\mathbf{r},\mathbf{r}')$ [here we leave aside the fact that for interacting systems, *no* Dirac-Fock ρ_0 can be equal to ρ], it is *not* possible unequivocally to establish the share of Σ^{GW} in the mentioned shortcoming of the associated spectral function. Our work (Farid 1994, 1997a) suggests, for instance, that a H_0 which produces accurate GS charge density, is likely to yield a $\Sigma^{GW}[G_0]$ according to which the fundamental QP gap is farther from the experimental value than that according to $\Sigma^{GW}[G_{KS-LDA}]$. In view of this and with reference to our discussions in Subsec. 9.8, we point out that it is most likely that for different applications — if one is to employ the SE operator within the GWA —, one needs to perform appropriately chosen types of self-consistent calculation, where the condition(s) to be met at self-consistency should be motivated by the nature of the application that one has in mind. It appears that as far as the energies of the low-lying single-particle excitations in semiconductors and insulators are concerned, the G_0 corresponding to the KS Hamiltonian within the LDA of the DFT qualifies as an "appropriate" choice with which to calculate $\Sigma^{GW}[G_0]$.

10. Summary and Concluding Remarks

In this work we have dealt with a number of basic elements from the theory of interacting fermions (specifically electrons). We have explicitly considered the single-particle Green function $G(\varepsilon)$, the SE operator $\Sigma(\varepsilon)$, the density-density correlation function $\chi(\varepsilon)$, the polarisation function $P(\varepsilon)$ and the pair-correlation function g (which by definition is independent of ε). We have analysed both some symmetry properties of these functions in the coordinate representation and their general behaviour as functions of the energy variable ε. We have given particular attention to two limits of the energy, those of small *and* large $|\varepsilon|$.

Since for $\varepsilon \to 0$ the density-density correlation function $\chi(\varepsilon)$ coincides with the functional derivative of the GS charge density n with respect to the *static* external potential v, and since n is *the* basic quantity within the framework of the GS density-functional theory (DFT), we have briefly outlined the salient features of this theory. Of particular relevance to the present work is that while the vertex function $\Gamma(1,2;3)$ pertaining to an inhomogeneous time-independent system is a function of *three* independent spatial coordinates and *two* independent energy (or time) variables, as far as the *static* χ is concerned, the influence of Γ is formally accounted for by an *energy-independent* function of *two* independent spatial variables. This function, $C(\mathbf{r},\mathbf{r}')$, is the first functional derivative of the effective Kohn-Sham (KS) potential with respect to the GS charge density (Subsubsec. 8.6.1). It must be emphasised that for such a C to exist, it is necessary that the GS charge density of the system under consideration is non-interacting v-representable (see Footnote 7).

That $\chi(\varepsilon)$ in the *static* limit, corresponding to $\varepsilon = 0$, is closely connected with the *ground-state* DFT, should not be surprising. However, that this is also the case for very large values of $|\varepsilon|$ (Subsecs. 8.3, 8.4 and 8.5), if not unexpected, is at least interesting. The same turns out to be the case for other correlation functions that we have considered in this work. By explicit calculation of the leading and next-to-leading asymptotic terms of these functions for $|\varepsilon| \to \infty$, we have established that these terms correspond to the GS properties that can in principle be addressed within the framework of the Hohenberg-Kohn-Sham DFT. Since the one-particle reduced density matrix ρ turns out to play a role in almost all asymptotic expressions that we have dealt with in the present work (those corresponding to the large-$|\varepsilon|$ limit), we have devoted some space to the discussion of two alternative KS (-type) formalisms in which the one-particle reduced density matrix plays a role.

Of these, one involves a Hartree–Fock-like, rather than the usual Hartree-like, KS equation. We have inferred (by relying upon a theorem that asserts that the exact ρ is *not* idempotent — see Footnote 99) that the Hartree–Fock-like KS framework[107] *cannot* be appropriate for yielding both the correct GS charge density and the exact one-particle reduced density matrix. However, we have established that the non-local exchange term that occurs in the KS Hamiltonian of this framework, is of some significance with regard to the behaviour of $\Sigma(\varepsilon)$ at large $|\varepsilon|$ (Subsec. 9.7). We have pointed out that as far as ρ is concerned, the appropriate density-functional framework is that first proposed by Gilbert (1975) — the exact one-particle reduced density matrix ρ within this framework is some ensemble average over the density matrices of a "non-interacting" KS Hamiltonian (see Footnote 78). We have not further discussed this framework in any detail. We can summarise our observations by stating that there exists some strong duality between the behaviour of correlation functions in the close vicinities of $\varepsilon = 0$ and $1/\varepsilon = 0$. This duality has far-reaching consequences, in particular for some fundamental aspects concerning the many-body perturbation theory (PT). We have only very briefly touched upon this subject in the present work.

Concerning the *dynamic* χ, with reference to the time-dependent DFT (Subsubsec. 8.6.2) we have pointed out that here, as in the static case, *in principle* an ε-dependent C operator can take account of the interaction effects that have not been accounted for by the dynamic density-density correlation function of a non-interacting KS system, $\chi_0(\varepsilon)$, described by a KS Hamiltonian. Owing to the fact that χ_0 is a *linear-response* function, the Hamiltonian to which $\chi_0(\varepsilon)$ corresponds is identical to the *ground-state* KS Hamiltonian. However, $C(\mathbf{r}, \mathbf{r}'; \varepsilon)$ cannot be defined for $|\varepsilon| > \varepsilon_{\min}$, with $\varepsilon_{\min}$ some finite (resonance) energy which is characteristic of the system under consideration.

Dynamic correlation functions pertaining to systems in the thermodynamic limit are peculiar: prior to taking the thermodynamic limit, it is *necessary* that the energy parameter ε in these functions be made complex valued, for otherwise in evaluating the limit, one encounters divergent contributions corresponding to ε being "pinched" by the adjacent poles located on the real axis.[108]

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[107] Originally proposed by Kohn and Sham (1965).

[108] Of course, *part* of the problem can be resolved by defining integrals (derived from infinite sums) to be principal-value integrals. This procedure fails however for singularities that coincide with the end points of the intervals of integration (as we have seen [Subsec. 2.4], these "end points" in reality turn into "branch points"). Further, the "imaginary" parts of the functions in question are not accounted for when integrals are simply replaced by principal-value integrals. See Footnote 70.

Once the energy parameter is made complex-valued, i.e. $\varepsilon \to z$ with $\mathrm{Im}(z) \neq 0$, the thermodynamic limit can be taken without any ill consequences. The process is not reversible, in that by letting $z \to \varepsilon$, with $\mathrm{Im}(\varepsilon) = 0$, one will *in general* not encounter poles on the real energy axis, but possibly branch points and branch cuts (Subsecs. 2.2 and 2.4). In fact, through a process of analytic continuation one can move from one half of the complex z-plane across the real axis into another half, bypassing the branch-cut discontinuity. The function that one thus obtains, provided the continuation has taken place through a branch-cut region, is a different branch of the original, i.e. physical, function. According to the terminology that we have adopted in this work, this new, i.e. unphysical, branch is referred to as the function in question "on a non-physical RS" (Subsec. 2.2). The many-valuedness of the correlation functions with which we have dealt in the present work, has in the main its root in the macroscopic nature of the systems under consideration.[100] Hence, we have extensively discussed the analytic properties of a number of correlation functions in the complex energy plane to which the *physical* correlation functions correspond through the process of analytic continuation. For instance $G(\varepsilon)$ is the limit of the function $\widetilde{G}(z)$ corresponding to $z = \varepsilon \pm i\eta$, with $\eta \downarrow 0$, where "+" is taken when $\varepsilon > \mu$ and "−" when $\varepsilon < \mu$; here μ stands for the "chemical potential" (see Subsec. 4.2). Without entering into details, we mention that an infinitesimal, but *non-vanishing*, η features in the formal theory of the many-body PT (see Subsec. 7.4): here by defining $\widehat{H}_\tau := \widehat{H}_0 + \exp(-\eta|\tau|/\hbar)(\widehat{H} - \widehat{H}_0)$, the interaction in $\widehat{H}_\tau$ is *adiabatically* (corresponding to $\eta \downarrow 0$) switched on and subsequently *adiabatically* switched off when τ is varied from $-\infty$ toward $+\infty$. The vital role played here by η for the realisation of the processes of (adiabatic) switching-on and switching-off of the interaction $\widehat{H} - \widehat{H}_0$, is equivalent with that played by η, with $\eta \downarrow 0$, in rendering such functions as $G(\varepsilon) := \widetilde{G}(\varepsilon \pm i\eta)$, $\varepsilon \gtrless \mu$, *physically* well-specified and meaningful.

The formal Lehmann and Lehmann-type representations for the dynamic correlation functions make explicit the physical significance of the singular points of these functions along the real energy axis. For example, the "poles"[110] of the single-particle GF are shown to correspond to the excitation energies associated with the energies of the $N \pm 1$-electron ground and excited states

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[109] For open systems, correlation functions have branch cuts even for finite number of particles. This is due to the fact that Hamiltonians of these systems in addition to a discrete set of energy levels possess a continuous spectrum.

[110] In the thermodynamic limit the designation "pole" may not apply — see Subsecs. 2.4, 6.1 and 8.7.

of the system with respect to the GS energy of the N-electron system; they correspond to the "single-particle excitation" energies. However, upon taking the limit $\eta \downarrow 0$ in $\widetilde{G}(\varepsilon \pm i\eta)$ pertaining to a system in the thermodynamic limit, it becomes apparent that *in general* at *no* point along the real ε-axis the function is unbounded.[111] Thus, the equations from which the mentioned excitation energies are to be obtained (the "quasi-particle equations") *in general* do not have solutions (Subsecs. 6.1 and 8.7). Possible solutions are to be sought on a non-physical RS, requiring analytic continuation of the pertinent functions (such as $\widetilde{\Sigma}(z)$ and $\widetilde{\chi}(z)$) across the branch cuts into the non-physical RSs.

The above inference has a number of consequences which we have discussed in some detail in the main text. First, in the thermodynamic limit, excitations in general do *not* correspond to one-particle stationary states of the many-electron system. Second, a solution of the quasi-particle (QP) equation on a non-physical RS corresponds to some superposition of a (macroscopically-) large number of stationary states of the interacting system. Such a one-particle-like excitation, a QP, *cannot* in consequence stand in any one-to-one correspondence with a single one-particle eigenstate of a non-interacting system. The assumption with regard to a one-to-one correspondence between the mentioned two states stands central in the *phenomenological* theory of Landau for Fermi liquids (Sec. 1).

The phenomenological Landau Fermi-liquid theory finds its theoretical justification within the framework of the many-body PT. Further, the phenomenological parameters that feature in Landau's theory can be determined in terms of the correlation functious pertaining to the interacting system, such as the single-particle GF. A characteristic feature of conventional Landau Fermi-liquid systems is the quadratic decrease of the imaginary part of the corresponding SE operators when the energy parameter ε approaches the Fermi energy (a Luttinger's theorem — Subsec. 6.4 and 6.5).[112] This implies that QPs in Fermi-liquid systems become the more well-defined the closer their energies are to the Fermi energy. Thus, on the Fermi surface of such systems, the QP excitations correspond to one-particle "stationary" states of the interacting Hamiltonian.[113]

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[111] This of course depends on the dimension of the spatial space; here we are mainly considering three-dimensional systems.

[112] With some modifications to this quadratic behaviour, one still may speak about a Landau Fermi liquid (Farid 1999a) — see Footnotes 47 and 52. We recall that a gapless effective non-interacting system, corresponding to an energy-*independent* Hermitian SE operator, is a Fermi liquid system — see Sec. 1.

[113] This is true in an asymptotic sense: as we have discussed in Subsec. 4.2, the singularity of $\widetilde{G}(\boldsymbol{k}; z)$ at $z = \mu_N$ is *not* an isolated singularity, and thus not a pole.

The mentioned behaviour of the SE operator in the close vicinity of the Fermi surface has some far-reaching consequences. One is a finite amount of discontinuity (less than unity) in the momentum distribution function at the Fermi momentum. The relationship between the magnitude of this discontinuity and the behaviour of $\Sigma(\varepsilon)$ for ε approaching the Fermi energy, is established by a celebrated theorem due to Migdal, which we have discussed in some detail in Subsec. 6.6. In doing so we have given particular attention to a number of delicate issues.

The above-indicated characteristic property concerning the imaginary part of the SE operator $\Sigma(\varepsilon)$ pertaining to (conventional) Fermi-liquid systems has been obtained within the framework of the many-body PT (Luttinger 1961, Luttinger and Ward 1960; see also Hugenholtz 1957, and DuBois 1959b). The behaviour of the SE operator for ε close to the Fermi energy is of vital influence on the thermodynamic as well as quasi-static transport properties of the corresponding systems at low temperatures. Therefore, a system whose low-temperature thermodynamic and quasi-static transport properties differ from those expected from the Landau Fermi liquids, must by implication correspond to a SE operator whose behaviour in the close vicinity of the Fermi energy is non-Fermi-liquid like. This deviation is often held as evidence for the breakdown of the many-body PT for the systems concerned (Subsecs. 6.4 and 6.5).

We have critically analysed the work by Luttinger (1961) which establishes Eq. (78). We have put forward a number of reasons to the effect that a non-Fermi-liquid behaviour does *not* necessarily imply breakdown of the many-body PT (Farid 1999a). The following is a summary of our analyses:

(i) All the diagrams treated by Luttinger involving polarisation insertions are individually divergent for systems of particles interacting through the long-range Coulomb interaction. For such systems, the diagrams must first be partially summed and expressed in terms of the dynamic *screened* interaction function. By doing so, the mathematical approach adopted by Luttinger can no longer be effective, following the fact that for this an *a priori* knowledge concerning the energies of the neutral excitations of the *interacting* N-electron system becomes indispensable. The difficulty in arriving at such a knowledge stands on a par with that in arriving at the knowledge with regard to the single-particle excitation energies of the *interacting* system that one has set out to determine in the first place.

(ii) Luttinger's generalisation of the results corresponding to skeleton SE diagrams in terms of the *non-interacting* GF to those in terms of the *interacting* GF, involves a *tacit assumption.* Neglecting for the time being the problem that we have indicated under point (i), the present point renders Luttinger's final result (presented in Eq. (78) of the present work) a mere *self-consistent* result: this result does not rule out other possible solutions (i.e., non-Fermi-liquid-like solutions) which by the mentioned tacit assumption are excluded.[114]

By demonstrating that the SE operator $\widetilde{\Sigma}(k;z)$ has branch points at $z = \mu_N$ (and $z = \mu_{N+1}$) — see Subsec. 4.2 —, we have shown that Eq. (78) cannot be the leading-order term for $\widetilde{\Sigma}''(k;z)$ corresponding to a Taylor series expansion of $\widetilde{\Sigma}(k;z)$ around $z = \mu_N$. Rather, the pertinent series for $\widetilde{\Sigma}(z)$ is a *divergent* asymptotic series expansion (Subsec. 2.3). Often insufficient distinction between what we have denoted by μ, μ_N and μ_{N+1}, with the property $\mu_N < \mu < \mu_{N+1}$ (see Subsec. 4.2), gives rise to mathematical and conceptual difficulties. Thus, whereas $\widetilde{\Sigma}(z)$ is singular at both $z = \mu_N$ and $z = \mu_{N+1}$, it is regular at $z = \mu$. Further, the above-mentioned asymptotic expansion for $\widetilde{\Sigma}(z)$ at $z = \mu_N$ (or $z = \mu_{N+1}$) is not a uniform one: it is different for two different sectors of the z-plane. The non-uniformity of this expansion is reflected in the branch cuts of $\widetilde{\Sigma}(z)$ along the real ε-axis which can be identified as the Stokes lines of $\widetilde{\Sigma}(z)$ (Subsec. 2.3) corresponding to these non-uniform asymptotic series.

We have enumerated a number of methods through which the single-particle GF corresponding the interacting system can be determined. From amongst these, we have given especial attention to the many-body PT. After a discussion concerning the possible problems from which this approach can suffer, we have indicated that provided the GS charge density of the system[115] be *pure-state non-interacting v-representable* (see Footnote 7), the many-body perturbation

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[114] We should like to point out that Luttinger (1960) in two places makes remarks that are relevant to our discussions here. After Eq. (51) in (Luttinger 1960), Luttinger remarks: "We have not succeeded in finding the necessary and sufficient conditions on the interaction between particles for which (51) [our Eq. (78)] is valid." Following Eq. (69) in (Luttinger 1960) one further finds: "what we have shown ... is that if we assume the property (51) we again obtain it, so that we have found a consistent solution." The "consistent solution" here is distinct from what above we have referred to as "*self-consistent* result". Incidentally, the pre-factor "u^2" in Eq. (60) of (Luttinger 1960) is a printing error; the correct pre-factor is unity.

[115] Recall that in the present work we have restricted our considerations to systems whose GSs are nondegenerate and spin-compensated (this includes systems of spin-less fermions with non-degenerate GSs). It is for this reason that the GS charge density plays such a prominent role in our present considerations.

expansion in terms of the associated KS Hamiltonian is unconditionally valid (Farid 1994, 1997a,b, 1999b). We have presented several indirect evidences in support of this statement. With reference to some arguments and examples put forward by Simon (1970), we have made explicit that criticisms raised against *the* many-body PT are often expressions of prevailing prejudices rather than outcomes of well-founded reasonings.

Indirect evidence that the KS Hamiltonian indeed should play a crucial role in the applications of the many-body PT, is abundant. Take for instance the asymptotic behaviour of the correlation functions pertaining to *interacting* systems that we have dealt with in the present work: invariably in all of these, for both $\varepsilon \to 0$ and $1/\varepsilon \to 0$, the GS charge density makes an appearance. It follows that, use of the "non-interacting" KS Hamiltonian in applications of the many-body PT has the effect that, in the mentioned limits, it is as if the many-body perturbation series were evaluated in terms of the *exact* GF of the interacting system. Our analyses further establish that, the "non-interacting" Hartree–Fock-like KS Hamiltonian (as distinct from the commonly-employed Hartree-like one — Subsec. 9.7) *may* be a better choice in applications of the many-body PT, as through it a certain contribution to the SE operator in the large-$|\varepsilon|$ limit is more accurately reproduced. For two reasons, however, this still falls short of being the absolute ideal choice (an "ideal" which of course is not achievable, at least not within the framework of our present work), namely (i) the single-particle reduced density matrix as determined within the Hartree–Fock-like KS formalism is a Dirac-Fock density matrix and therefore cannot be identical with that of the interacting system; (ii) the Hartree–Fock-like KS Hamiltonian involves a local correlation potential, i.e. v_c, which does not explicitly occur in the large-$|\varepsilon|$ asymptotic series expansions of correlation functions. We have to pointed out (Subsec. 9.7) that the appropriate theoretical formalism for determination of ρ pertaining interacting systems is the DFT for non-local external potentials, first put forward by Gilbert (1975); see also Donnelly and Parr (1978) and Valone (1980). However, a direct application of this formalism within the many-body PT is hampered by the fact that ρ in Gilbert's approach corresponds to an *ensemble* of the many-body eigenstates of a "non-interacting" KS Hamiltonian (see Footnote 78).

We have discussed in considerable detail an approximate form of the SE operator Σ, namely the first-order term in the expansion of Σ in terms of the dynamic screened interaction function W. Since this SE operator involves one single-particle Green function G and one W, it is usually referred to as the *GW* approximation (GWA) to Σ, Σ^{GW}. We have analysed various aspects of Σ^{GW}. Through detailed examination of the behaviour of $\Sigma^{GW}(\varepsilon)$ for large $|\varepsilon|$, we have established the conditions under which a $\Sigma^{GW}[G_0]$ (i.e. Σ^{GW} evaluated in terms of a G_0 — Subsecs. 7.6 and 9) can have an asymptotic behaviour similar to $\Sigma^{GW}[G]$. From this, we have once more arrived at the conclusion that in general use of the KS Hamiltonian, and thus of the corresponding G_0 and W^{RPA} (see Subsec. 8.5), leads to the most favourable outcome.[116] We have elaborated on a number of technical issues that are of relevance to the evaluation of Σ^{GW} in practical applications. Further, we have discussed a number of strategies concerning self-consistent evaluation of Σ^{GW}. A brief exposition of a number of research articles which in the main are concerned with the application of the GWA to real materials, is presented in Subsec. 9.10. Limitation of space has prevented us from discussing these works in any depth. We have, however, presented a concise account of what may be considered as "general trends" in the computed results, as well as some aspects that experience has shown to be of utmost significance for rendering the GWA a reliable scheme.

To summarise the entire work, we have considered a number of *relatively* simple interdependent (dynamic) correlation functions, determination of each of which necessitates that of the rest. Therefore, although limited in scope, this work provides a reasonably detailed account of a number of elements of the theory of many-particle systems that are basic to addressing problems in which electron-electron interaction plays a role. We have examined a number of properties of the mentioned correlation functions, and attempted *explicitly* to expose some of the deep, and thus hidden, connections between some properties of the GS and those of the excited states. This has enabled us directly to indicate the important role that the KS Hamiltonian (in its various forms appropriate to specific problems) can play within the framework of the many-body PT. Our incomplete knowledge with regard to the explicit dependence of this Hamiltonian on the GS charge density (see Footnote 115) necessitates determination of this Hamiltonian within a self-consistent scheme. Elsewhere we have proposed and applied (Farid 1994, 1997a,b, 1999b) a self-consistent scheme for the determination of this Hamiltonian. The numerical results obtained within this scheme are extremely satisfying. The work that we have

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[116] It should be pointed out that G_{KS} implicitly depends on v_c, and this dependence is highly non-perturbative. A perturbation series in terms of G_{KS} is therefore *not* a power series in the coupling constant of the electron-electron interaction.

presented here further brings out the importance of analysing the asymptotic behaviour of correlation functions in regions $\varepsilon \to 0$ and $|\varepsilon| \to \infty$ when explicit calculations of these functions are being considered.

Appendix A: On the representation spaces and some conventions

Here we present the various representations that we encounter in this work. We restrict ourselves to systems in the thermodynamic limit.

As a typical example of a correlation function, consider the single-particle Green *function* $G(\mathbf{r}, \mathbf{r}'; \varepsilon)$. This function is the coordinate representation of the Green *operator* $G(\varepsilon)$. Thus $G(\mathbf{r}, \mathbf{r}'; \varepsilon) := \langle \mathbf{r}|G(\varepsilon)|\mathbf{r}'\rangle$, where $|\mathbf{r}\rangle$ and $|\mathbf{r}'\rangle$ are normalised eigenstates of the $\widehat{\mathbf{r}}$ operator; we have $\widehat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle$, with $\langle \mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r} - \mathbf{r}')$. In the same spirit, $G(\mathbf{k}, \mathbf{k}'; \varepsilon)$ stands for $\langle \mathbf{k}|G(\varepsilon)|\mathbf{k}'\rangle$, where $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$ are normalised eigenstates of the one-particle wave-vector operator, $\widehat{\mathbf{k}}|\mathbf{k}\rangle = \mathbf{k}|\mathbf{k}\rangle$, with $\langle \mathbf{k}|\mathbf{k}'\rangle = \delta_{\mathbf{k},\mathbf{k}'}$.[117] We have $\langle \mathbf{r}|\mathbf{k}\rangle = \Omega^{-1/2} \exp(i\mathbf{k} \cdot \mathbf{r})$. In a crystal, where, e.g., $G(\mathbf{r} + \mathbf{R}, \mathbf{r}' + \mathbf{R}; \varepsilon) = G(\mathbf{r}, \mathbf{r}'; \varepsilon)$, for any *primitive* translation vector $\mathbf{R}$ of the underlying Bravais lattice, we have $G(\mathbf{k}, \mathbf{k}'; \varepsilon) \equiv 0$ unless $\mathbf{k} - \mathbf{k}' = \mathbf{K}$, with $\mathbf{K}$ *some* RLV associated with the mentioned lattice. We therefore ignore all these symmetry-bound zero matrix elements and denote the remaining matrix elements by $G_{\mathbf{G},\mathbf{G}'}(\mathbf{k}; \varepsilon)$ which is the short for $G(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G}'; \varepsilon)$. Here $\mathbf{G}$ and $\mathbf{G}'$ are RLVs and $\mathbf{k}$ is restricted to lie inside the first Brillouin zone (1BZ). For a given $\mathbf{k} \in$ 1BZ, $\{|\mathbf{k}+\mathbf{G}\rangle\}$ satisfies the normalisation condition, $\langle \mathbf{k} + \mathbf{G}|\mathbf{k} + \mathbf{G}'\rangle = \delta_{\mathbf{G},\mathbf{G}'}$. In these systems, by choosing the one-body functions (the "wavefunctions") to be simultaneously basis functions of the unitary irreducible representations of the underlying lattice translation group of the Hamiltonian (Cornwell 1984, pp. 81–83), the index s attached to such functions as $\widetilde{\psi}_s(\mathbf{r}; z)$ can be replaced by the pair of indices $(\ell, \mathbf{k})$, with $\mathbf{k} \in$ 1BZ, and ℓ a "band index"; $\widetilde{\psi}_{\ell,\mathbf{k}}(\mathbf{r}; z)$, a Bloch function, is then said to transform according to the $\mathbf{k}$ irreducible representation of the underlying lattice translation group. In the extended-zone representation, where $\mathbf{k}$ extends over the whole reciprocal space, time-reversal symmetry implies that if $s \leftrightarrow \mathbf{k}$, then $\overline{s} \leftrightarrow -\mathbf{k}$. The association $s \leftrightarrow (\ell, \mathbf{k})$, does *not* imply $\overline{s} \leftrightarrow (\ell, -\mathbf{k})$, however, following the fact that indices of the "bands" at different points inside

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[117] In the solid-state physics it is customary separately to consider the momentum vector $\mathbf{p}$ and the corresponding wave-vector $\mathbf{k} \equiv \mathbf{p}/\hbar$. Note that, here we employ the "box" boundary condition, so that the allowed wave vectors form a discrete set and whereby $(2\pi)^3\delta(\mathbf{k} - \mathbf{k}')/\Omega \leftrightarrow \delta_{\mathbf{k},\mathbf{k}'}$, where Ω denotes the macroscopic volume of the system (in works concerning systems in d spatial dimensions, 3 in $(2\pi)^3$ changes into d).

the 1BZ need not be related; $s \leftrightarrow (\ell, \mathbf{k})$ implies that there exists *an* ℓ' such that $\bar{s} \leftrightarrow (\ell', -\mathbf{k})$; when "bands" are not disrupted by gaps, it is possible, by means of an analysis of the symmetries of the states at different **k**-points (this is the so-called "compatibility analysis"), to assign indices to the bands in such a way that $s \leftrightarrow (\ell, \mathbf{k})$ indeed implies $\bar{s} \leftrightarrow (\ell, -\mathbf{k})$. Making use of the representations $\widetilde{\psi}_{\ell,\mathbf{k}}(\mathbf{r}; z) = \exp(i\mathbf{k} \cdot \mathbf{r})\widetilde{u}_{\ell,\mathbf{k}}(\mathbf{r}; z)$ and $\widetilde{\phi}_{\ell,\mathbf{k}}(\mathbf{r}; z) = \exp(i\mathbf{k} \cdot \mathbf{r})\widetilde{v}_{\ell,\mathbf{k}}(\mathbf{r}; z)$, with $\widetilde{u}_{\ell,\mathbf{k}}$ and $\widetilde{v}_{\ell,\mathbf{k}}$ periodic functions of **r**, from Eqs. (58) and (59), making use of $\widetilde{\Sigma}(\mathbf{r}, \mathbf{r}'; z) = \widetilde{\Sigma}(\mathbf{r}', \mathbf{r}; z)$ in Eq. (40), the result concerning the Kramers degeneracy of states (Landau and Lifshitz 1977, pp. 223–226, Callaway 1964, pp. 52–54; see Footnote 21), namely $\widetilde{E}_{\ell,\mathbf{k}}(z) = \widetilde{E}_{\ell',-\mathbf{k}}(z)$, can be directly verified.

For systems with continuous translation symmetry,[118] $G(\mathbf{r}, \mathbf{r}'; \varepsilon)$ is a function of $\|\mathbf{r} - \mathbf{r}'\|$. Dependence on $\mathbf{r} - \mathbf{r}'$ implies that $G(\mathbf{k}, \mathbf{k}'; \varepsilon) \equiv 0$ unless $\mathbf{k} = \mathbf{k}'$. The dependence on the norm of $\mathbf{r} - \mathbf{r}'$ further implies that $G(\mathbf{k}, \mathbf{k}; \varepsilon)$ is a function of $k := \|\mathbf{k}\|$, with $k \in [0, \infty)$. For these reasons, for spatially uniform systems we employ the notation $G(k; \varepsilon)$.

Appendix B: Discontinuity in the Time Domain versus Asymptotic Behaviour in the Energy Domain

In this Appendix we demonstrate some close connections between the behaviour of $f(t)$ for $|t| \to 0$ and that of its Fourier transform $F(\varepsilon)$ for $|\varepsilon| \to \infty$. In view of our extensive analyses with regard to the large-$|\varepsilon|$ behaviour of various correlation functions, exposition of these connections should prove interesting.

First we recall that $\theta(t) = i\hbar \int_{-\infty}^{\infty} d\varepsilon/(2\pi\hbar) \exp(-i\varepsilon t/\hbar)/(\varepsilon + i\eta)$, $\eta \downarrow 0$. Now consider $F(\varepsilon)$ whose leading asymptotic term for $|\varepsilon| \to \infty$ is of the form a/ε, with a independent of ε. By adding and subtracting $a/(\varepsilon + i\eta)$ from $F(\varepsilon)$, making use of the above representation for $\theta(t)$ and the relation $1/(\varepsilon + i\eta) = \mathcal{P}(1/\varepsilon) - i\pi\delta(\varepsilon)$, with $\mathcal{P}$ the Cauchy principal value, we obtain

$$f(t) = -\frac{ia}{2\hbar}\,\mathrm{sgn}(t) + \mathcal{P}\int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi\hbar} \left\{F(\varepsilon) - \frac{a}{\varepsilon}\right\} \exp(-i\varepsilon t/\hbar)\,. \tag{B.1}$$

Since by definition $\varepsilon(F(\varepsilon) - a/\varepsilon) = o(1)$ when $|\varepsilon| \to \infty$, say $(F(\varepsilon) - a/\varepsilon) \sim b/\varepsilon^{\alpha}$ with $\alpha > 1$ and b a constant with respect to ε, it follows that the last term

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[118] Because of the assumed non-degeneracy of the GS, this symmetry, which is that of the many-body Hamiltonian, is also the symmetry of the GS.

on the RHS of Eq. (B.1) is a continuous function of t. This is a consequence of the fact that the principal-value integral of the term inside the curly braces converges *uniformly* (Whittaker and Watson 1927, pp. 75 and 70, Titchmarsh 1939, p. 22) and that $\exp(-i\varepsilon t/\hbar)$ is *continuous* everywhere (see Whittaker and Watson 1927, p. 73); the principal-value sign implies that the infinitesimal neighbourhood of $\varepsilon = 0$ is not part of the integration region. Thus we observe that the discontinuous part of $f(t)$, i.e. the first term on the RHS of Eq. (B.1), is entirely determined by the coefficient a of the $(1/\varepsilon)$-term in the asymptotic expansion of $F(\varepsilon)$ for $|\varepsilon| \to \infty$ (the imaginary unit i reflects the fact that asymptotically $F(\varepsilon)$ behaves like an *odd* function of ε). Along the same lines we can prove the following general statements: Let $F(\varepsilon) \sim a/\varepsilon^n$ for $|\varepsilon| \to \infty$, with a a non-zero constant with respect to ε and n some positive integer. Then (when $n-2 \geq 0$) $\partial^{n-2} f(t)/\partial t^{n-2}$ is continuous at $t=0$ and (when $n-1 \geq 0$) $\partial^{n-1} f(t)/\partial t^{n-1}$ has a *finite* discontinuity at $t=0$.

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LIST OF SOME SYMBOLS

$\equiv$	$f(x) \equiv g(x)$, f and g are *identical* over the entire range of definition
$:=$	$f(x) := g(x)$, f is *defined* according to g, i.e. $f(x)$ is *by definition* equal to $g(x)$
$=:$	$f(x) =: g(x)$, g is *defined* according to f
$\sim$	$f(x) \sim g(x)$ for $x \to x_0$ (say, $x_0 = \infty$), $f(x)$ is asymptotically equivalent with $g(x)$, i.e. $f(x)/g(x) \to 1$ when $x \to x_0$
$\sim'$	$f(x) \sim' g(x)$, for $x \to x_0$; similar to $f(x) \sim g(x)$ *except* that $f(x)/g(x) \to C$ when $x \to x_0$, with C independent of x
$\propto$	$f(x) \propto g(x)$, f is proportional to g for *all* x
$\cong$	$f \cong g$, f approaches g in the thermodynamic limit
$\approx$	$f \approx g$, f is *approximately* equal to g
$\to$	$x \to x_0$, x approaches x_0
$\simeq$	$M \simeq m$, M is on the order of m
$\downarrow$	$\eta \downarrow 0$, η approaches 0 from above, i.e. η is positive infinitesimal
$\Longleftrightarrow$	$S_1 \Longleftrightarrow S_2$, statement S_1 implies statement S_2 and *vice versa*
$\leftrightarrow$	$a \leftrightarrow b$, within a particular context b is to be identified with a
$\mathcal{O}$	A Landau's symbol (E.G.H. Landau); $f(x) = \mathcal{O}(g(x))$, there exists a constant C such that $\vert f(x)\vert \leq C\vert g(x)\vert$
o	A Landau's symbol (E.G.H. Landau); $f(x) = o(g(x))$ for $x \to x_0$ implies $f(x)/g(x) \to 0$ for $x \to x_0$
$\Vert\cdot\Vert$	Cartesian norm; *c.f.* $\Vert\mathbf{r}\Vert =: r \equiv (x^2 + y^2 + z^2)^{1/2}$
ε	Real-valued energy parameter
z	Complex-valued energy parameter; unless otherwise stated, $\mathrm{Im}(z) \neq 0$
$\varepsilon', \varepsilon''$	Real and imaginary parts of z, $z = \varepsilon' + i\varepsilon''$
$\widetilde{f}(z)$	Analytic continuation of $f(\varepsilon)$ into the *physical* Riemann sheet; *c.f.* $\Sigma(\varepsilon)$ and $\widetilde{\Sigma}(z)$
$\widetilde{\widetilde{f}}(z)$	Analytic continuation of $f(\varepsilon)$ or $\widetilde{f}(z)$ into a *non-physical* Riemann sheet; *c.f.* $\widetilde{\Sigma}(z)$ and $\widetilde{\widetilde{\Sigma}}(z)$
$\mathcal{F}(z)$	Unless otherwise stated, union of $f(\varepsilon)$, $\widetilde{f}(z)$ and *all* $\widetilde{\widetilde{f}}(z)$
$\widetilde{O}'(z)$	$\widetilde{O}'(z) := \frac{1}{2}\{\widetilde{O}(z) + \widetilde{O}^{\dagger}(z)\}$; *c.f.* $\widetilde{\chi}'(z)$

$\widetilde{O}''(z)$	$\widetilde{O}''(z) := \frac{1}{2i}\{\widetilde{O}(z) - \widetilde{O}^{\dagger}(z)\}$; *c.f.* $\widetilde{\chi}''(z)$
I	Unit operator (in a space to be specified, explicitly or implicitly)
$[a, b]$	Closed interval between a and b; $x \in [a, b]$ implies $a \leq x \leq b$
$[a, b)$	Semi-closed interval between a and b; $x \in [a, b)$ implies $a \leq x < b$
$(a, b]$	Semi-closed interval between a and b; $x \in (a, b]$ implies $a < x \leq b$
(a, b)	Open interval between a and b; $x \in (a, b)$ implies $a < x < b$

LIST OF ABBREVIATIONS AND ACRONYMS

1BZ	The first Brillouin zone
BZ	Brillouin zone
DFT	Density-functional theory
DOS	Density of states
EOM	Equation of motion
GF	Green function; if not explicitly specified, the single-particle GF
GS	Ground state
GWA	GW approximation for the self-energy operator
KS	Kohn-Sham
LDA	Local-density approximation
LHS	Left-hand side
PT	Perturbation theory
QP	Quasi particle
RHS	Right-hand side
RLV	Reciprocal lattice vector
RPA	Random-phase approximation
RS	Riemann sheet
SE	Self-energy

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