

Analysis of exact vertex function for improving on the GW scheme for first-principles calculation of electron self-energy

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In order to propose a sophisticated scheme for the self-consistent calculation of the electron self-energy Σ , a detailed analysis of the analytical structure of the three-point vertex function Γ is made with full respect for the Ward identity from the perspective of Fermi-liquid theory. Our scheme may be regarded as an improvement on the gauge-invariant self-consistent approximation to the exact theory for obtaining Σ as a fixed point of the self-energy revision operator \mathcal{F} , indicating an intrinsically nonperturbative approach applicable to both Fermi and Tomonaga-Luttinger liquids in a unified manner, but it may also be considered as providing a general framework for constructing an accurate functional form for Γ in the GW method for the first-principles calculation of Σ . Our result on the momentum distribution function in the homogeneous electron gas is compared with the one recently obtained by the reptation Monte Carlo method.

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I. INTRODUCTION

The electron self-energy $\Sigma(\mathbf{k}, \omega)$ is a fundamental quantity in the Green's function approach to the many-electron problem in solids. It is directly related to the one-electron spectral function $A(\mathbf{k}, \omega)$ that can be observed experimentally by angle-resolved photoemission spectroscopy (ARPES). Accurate information on $\Sigma(\mathbf{k}, \omega)$ in a wide range of momentum \mathbf{k} and energy ω is useful not only for elucidating the detailed Fermi-liquid properties in usual metals but also for discussing the non-Fermi-liquid behavior inherent to the Tomonaga-Luttinger liquid (TLL) in systems with one spatial dimension.^{1,2}

In 1965, Hedin formulated a formally rigorous framework to determine the exact self-energy Σ_{exact} by deriving a closed set of equations (Hedin's equations) to connect Σ with the one-electron Green's function G , the dynamically screened interaction W , the polarization function Π , and the three-point vertex function Γ .³ In practice, however, we cannot faithfully implement this formulation, because we cannot obtain the electron-hole irreducible interaction \tilde{I} , a key quantity in the Bethe-Salpeter equation to give the exact vertex function Γ_{exact} , through its original definition using a functional derivative, $\tilde{I} \equiv \delta\Sigma/\delta G$. Under this circumstance, Hedin considered a perturbation expansion in terms of W and advocated the usefulness of its lowest order term or the GW approximation (GWA) to Σ , in which Γ is taken as unity.

This GWA is a conserving approximation in the Baym-Kadanoff's sense,^{4,5} obeying the conservation laws of the *macroscopic* quantities such as the total electron number, but because of the omission of all vertex corrections it does not satisfy the Ward identity (WI),^{6,7} an exact relation between Σ and Γ due to gauge invariance representing the *local* electron-number conservation. Under the violation of the WI, we cannot expect to obtain an accurate enough Σ in Fermi-liquid metals.^{8,9} In TLL metals, the situation about the GWA becomes even worse, because a perturbative approach to Hedin's theory is inappropriate from the outset for describing the nonperturbative features of the TLL.

In 1995, one of the authors (Y.T.) demonstrated that Hedin's equations could be solved nonperturbatively by introducing

“the self-energy revision operator” \mathcal{F} .^{10,11} This operator \mathcal{F} is so defined as to operate on an arbitrary input self-energy Σ_{input} to produce an output self-energy Σ_{output} as

$$\Sigma_{\text{output}} = \mathcal{F}[\Sigma_{\text{input}}], \quad (1)$$

in which we include Γ as a solution to the Bethe-Salpeter equation with the integral kernel $\tilde{I}_{\text{input}} \equiv \delta\Sigma_{\text{input}}/\delta G$, which is not the same as the exact \tilde{I} , so that this Γ , the central quantity in the definition of \mathcal{F} , satisfies the WI in conjunction with not Σ_{exact} but Σ_{input} . Then it is proved that the exact self-energy Σ_{exact} is characterized as a “fixed point” of this revision operator \mathcal{F} , i.e., $\Sigma_{\text{exact}} = \mathcal{F}[\Sigma_{\text{exact}}]$, indicating that an iterative algorithm is very useful in obtaining Σ_{exact} in this self-energy revision operator theory. Here we emphasize that this is not a procedure to make diagram-by-diagram inclusion of higher order terms in Σ but an algorithm in which by simply operating \mathcal{F} repeatedly on an initial Σ_{input} (which we may give at our disposal), all higher order terms are automatically and appropriately included without the problem of double counting, as clearly discussed in Ref. 10 as the most prominent feature of this theory.

Contrary to the exact \tilde{I} , \tilde{I}_{input} can be calculated exactly, as long as Σ_{input} is concretely specified as a functional of G , but for making actual implementation of the iterative algorithm feasible, we had better avoid determining Γ by explicitly solving the Bethe-Salpeter equation with \tilde{I}_{input} under a given Σ_{input} at each iteration step. It is, rather, recommended to employ a predetermined functional for Γ , $\Gamma[\Sigma_{\text{input}}]$, which is a functional of Σ_{input} and possibly along with other quantities such as G that are easily derived from Σ_{input} . Thus it is the crux in our iterative algorithm to develop an accurate enough, if not exact, $\Gamma[\Sigma_{\text{input}}]$ for an arbitrary Σ_{input} . In this development, it is natural to think of exploiting the exact relation of the WI between Γ and Σ_{input} . In fact, as early as 1993, the simplest approximate form for $\Gamma[\Sigma_{\text{input}}]$ with use of only the WI was proposed and named the gauge-invariant self-consistent (GISC) method.¹² This GISC scheme, however, does not work very well in metals due primarily to the insufficient treatment of the so-called q limit in the Fermi-liquid theory.^{10,13,14}

In pursuing a further developed functional form beyond the GISC scheme, we should keep in mind that Γ_{exact} will be well approximated by $\Gamma[\Sigma_{\text{exact}}]$, if $\Gamma[\Sigma_{\text{input}}]$ is actually obtained as an appropriate one for an *arbitrary* Σ_{input} . Putting it in a reverse way, we should recognize that the functional form will never be very much improved without a detailed study of the analytical structure of Γ_{exact} . Thus in this paper, from the perspective of Fermi-liquid theory, we shall do such an analysis as the main issue with a view to constructing a good functional form for $\Gamma[\Sigma_{\text{input}}]$. This functional turns out to be valid for both Fermi-liquid and TLL metals.

Incidentally, if we obtain a good $\Gamma[\Sigma]$ for Σ in the “neighborhood” of Σ_{exact} in the abstract space of self-energy functions $\{\Sigma\}$ on which \mathcal{F} operates, we can avail ourselves of the same functional in the GW Γ scheme for the first-principles calculation of the electron self-energy. The GW Γ scheme is not necessarily couched on the self-energy revision operator theory and in fact a few different versions have been proposed so far.^{8,15,16} Among them, the WI is satisfied only in the one proposed in Ref. 8, in which a rather good form for $\Gamma[\Sigma]$ has been proposed with the introduction of the concept of “the ratio function” and successfully applied to the three-dimensional (3D) homogeneous electron gas at metallic densities. This version of the GW Γ scheme, however, encounters a serious problem in the electron gas with densities lower than the metallic ones: Convergent results for Σ are not obtained, if its density specified by the dimensionless parameter r_s is larger than 5.25 where there appears the dielectric catastrophe associated with the divergence of the compressibility κ at $r_s = 5.25$ and concomitantly that of the static polarization function Π in the long-wavelength limit.^{17–19}

In view of the above-mentioned success and failure, we shall revise the GW Γ scheme not only by giving $\Gamma[\Sigma]$ better than that in Ref. 8 but also by modifying the scheme itself into one free from the difficulty originating from the dielectric catastrophe. Furthermore, we shall propose a scheme for obtaining Σ alternative to the GW Γ one on the condition that an accurate piece of information is available for Π by other calculations or experiments. The proposal of these kinds of revisions and improvements constitutes another important issue of this paper.

This paper is organized as follows: In Sec. II we begin with specifying the Hamiltonian H for a translationally invariant system with which we are mainly concerned here. Then we concretely write down Hedin’s equations, together with the WI and related exact relations, pertinent to the system described by H . In Sec. III we analyze the analytical structure of the exact vertex function for small transferred momentum and frequency from the viewpoint of Fermi-liquid theory. Based on this analysis we propose a rather general functional form for the vertex function valid for both Fermi and Tomonaga-Luttinger liquids. In Sec. IV we extrapolate the functional form thus derived for the small momentum-frequency transfer to the one appropriate in the whole momentum-frequency space. Then we employ it in the GW Γ scheme to obtain its improved version, in which the iteration loop is modified into the one dubbed the G $\tilde{W}\tilde{\Gamma}_{\text{WI}}$ scheme. As an example to illustrate the power of this G $\tilde{W}\tilde{\Gamma}_{\text{WI}}$ scheme, the results are given for both $A(\mathbf{k},\omega)$ and the momentum distribution function $n(\mathbf{k})$ in the low-density electron gas with r_s up to 8. Before concluding

this section, we make several comments on various aspects, including the comparison of our result for $n(\mathbf{k})$ with the one recently obtained by the reptation Monte Carlo method²⁰ and an interesting piece of crossover behavior of the quasiparticle effective mass m^* in comparison with the bare one m with the increase of the quasiparticle momentum k in the electron gas at $r_s = 8$. In Sec. V an alternative to the GW Γ scheme is proposed, if Π is accurately known by some other methods. The results obtained in this paper are summarized in Sec. VI. We shall employ units in which $\hbar = k_B = 1$.

II. PRELIMINARIES

A. Hamiltonian

The algorithm we shall propose can be applied equally well to both fermions and bosons. It can also be used for inhomogeneous as well as homogeneous systems. We can employ it even for the electron-phonon systems, but for simplicity we confine ourselves to treating a homogeneous gas of n electrons in a unit volume interacting with one another through a two-body potential in this paper.

In these circumstances, the Hamiltonian we consider is written in second quantization as

$$H = H_0 + V, \quad (2)$$

with

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \quad (3)$$

and

$$V = \frac{1}{2} \sum_{\mathbf{q}} \sum_{\mathbf{k},\sigma} \sum_{\mathbf{k}',\sigma'} V(\mathbf{q}) c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}'-\mathbf{q}\sigma'}^\dagger c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma}, \quad (4)$$

where $c_{\mathbf{k}\sigma}$ is the annihilation operator of an electron with momentum \mathbf{k} and spin σ whose single-particle energy is given by $\epsilon_{\mathbf{k}} \equiv \mathbf{k}^2/2m$ with the mass of an electron m and $V(\mathbf{q})$ is the Fourier transform of a two-body interaction potential. No specific form is needed for $V(\mathbf{q})$, but in considering the application to the electron gas in Sec. IV, $V(\mathbf{q})$ will be taken as $4\pi e^2/\mathbf{q}^2$. In principle, no restrictions are imposed on spatial dimensions, but we study three-dimensional systems in this paper. (One- and two-dimensional systems will be discussed elsewhere.)

B. Hedin’s equations

Let us start with recapitulating the exact relations for interacting-electron systems with translational symmetry in which momentum is a good quantum number. The Dyson equation relates the one-electron thermal Green’s function $G(K)$ with the self-energy $\Sigma(K)$ through

$$G(K) = \frac{1}{i\omega_k + \mu - \epsilon_{\mathbf{k}} - \Sigma(K)}, \quad (5)$$

where μ is the chemical potential, $K \equiv \{\mathbf{k}, \omega_k\}$ is a combined notation of momentum \mathbf{k} and fermion Matsubara frequency ω_k defined at a temperature T .

The Bethe-Salpeter equation determines the proper non-dimensional three-point vertex function $\Gamma^\nu(K, K + Q)$ in a charge channel as

$$\begin{aligned} \Gamma^\nu(K, K + Q) &= \gamma^\nu(K, K + Q) \\ &+ 2 \sum_{K'} \tilde{I}(K, K + Q; K', K' + Q) \\ &\times G(K')G(K' + Q)\Gamma^\nu(K', K' + Q), \quad (6) \end{aligned}$$

for $\nu = 0$ (scalar part) and $\nu = 1$ (longitudinal vector part), where $Q \equiv \{\mathbf{q}, \omega_q\}$ is a notation combining momentum \mathbf{q} and boson Matsubara frequency ω_q , $\sum_{K'}$ is a shorthand notation for the sum over $\omega_{k'}$ and the integral over \mathbf{k}' , namely, $\sum_{K'} = T \sum_{\omega_{k'}} \int d^3k' / (2\pi)^3$, the factor 2 in front of the sum takes care of the spin degree of freedom, and $\tilde{I}(K, K + Q; K', K' + Q)$ is the electron-hole irreducible four-point interaction in the charge channel. The bare three-point vertex for the scalar part is defined as $\gamma^0(K, K + Q) = 1$, while the one for the longitudinal vector part in the non-dimensional form is introduced as $\gamma^1(K, K + Q) = (\mathbf{q}/q) \cdot [(\mathbf{k} + \mathbf{q}/2)/m] / v_F = (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) / v_F q$ with $q \equiv |\mathbf{q}|$ and the Fermi velocity $v_F \equiv k_F/m \equiv |\mathbf{k}_F|/m$, where \mathbf{k}_F is the Fermi momentum, related to the electron number density n through $n = k_F^3/3\pi^2$.

In terms of these three-point vertex functions, we may define the polarization function $\Pi^{\nu\nu'}(Q)$ by

$$\begin{aligned} \Pi^{\nu\nu'}(Q) &= -2 \sum_K \gamma^\nu(K, K + Q) \\ &\times G(K)G(K + Q)\Gamma^{\nu'}(K + Q, K). \quad (7) \end{aligned}$$

It is easy to confirm a symmetric relation $\Pi^{01}(Q) = \Pi^{10}(Q)$ from Eqs. (6) and (7), which may be recognized as one of the Onsager relations.

Once the polarization function $\Pi^{00}(Q)$ is known, the dynamically screened interaction $W(Q)$ is obtained as

$$\begin{aligned} W(Q) &= V(\mathbf{q}) - V(\mathbf{q})\Pi^{00}(Q)W(Q) \\ &= V(\mathbf{q})/[1 + V(\mathbf{q})\Pi^{00}(Q)]. \quad (8) \end{aligned}$$

By using $W(Q)$, together with G and Γ^0 , we can write down the equation to determine the self-energy $\Sigma(K)$ as

$$\Sigma(K) = - \sum_Q W(Q)\Gamma^0(K + Q, K)G(K + Q), \quad (9)$$

where \sum_Q denotes the sum over the variable Q ; i.e., $\sum_Q \equiv T \sum_{\omega_q} \sum_{\mathbf{q}} = T \sum_{\omega_q} \int d^3q / (2\pi)^3$.

The above five equations, Eqs. (5)–(9), constitute Hedin's closed set of equations to determine the self-consistent electron self-energy $\Sigma(K)$. Since both G and $\tilde{I}(=\delta\Sigma/\delta G)$ may be considered as functionals of Σ , Γ^ν in Eq. (6) is regarded as a functional of Σ as well, allowing us to write $\Gamma^\nu[\Sigma]$. With a good knowledge of $\Gamma^0[\Sigma]$, Hedin's set of equations can actually be solved numerically to give a concrete form of $\Sigma(K)$. The simplest form for this functional is, of course, $\Gamma^0[\Sigma] = 1$, as is the case in the GWA, but the main purpose of this paper is to propose a much systematically improved functional form for $\Gamma^0[\Sigma]$ by the consideration of its analytical structure.

C. Ward identity and related exact relations

The electron density operator $\rho(\mathbf{r}, t)$ is directly related to the electron current density operator $\mathbf{j}(\mathbf{r}, t)$ through the continuity equation, $\partial\rho(\mathbf{r}, t)/\partial t + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0$, representing the local conservation of electron number. With use of this relation, we can derive the Ward identity (WI) to connect the vertex functions, $\Gamma^0(K, K + Q)$ and $\Gamma^1(K, K + Q)$, with the one-electron Green's function as

$$\begin{aligned} i\omega_q \Gamma^0(K, K + Q) - v_F q \Gamma^1(K, K + Q) \\ = G^{-1}(K + Q) - G^{-1}(K). \quad (10) \end{aligned}$$

Note that $\Gamma^1(K, K + Q)$ is normalized in units of v_F here.

By substituting Eq. (10) into Eq. (7), we obtain a couple of equations for $\Pi^{\nu\nu'}(Q)$ as

$$\begin{aligned} i\omega_q \Pi^{00}(Q) - v_F q \Pi^{01}(Q) \\ = -2 \sum_{\mathbf{k}} [n(\mathbf{k}) - n(\mathbf{k} + \mathbf{q})] = 0, \quad (11a) \end{aligned}$$

$$\begin{aligned} i\omega_q \Pi^{10}(Q) - v_F q \Pi^{11}(Q) \\ = -2 \sum_{\mathbf{k}} \frac{\epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}-\mathbf{q}} - 2\epsilon_{\mathbf{k}}}{v_F q} n(\mathbf{k}) = -\frac{D_F}{3} v_F q, \quad (11b) \end{aligned}$$

where $n(\mathbf{k})$ is the interacting-electron momentum distribution function, given by $n(\mathbf{k}) = T \sum_{\omega_k} G(K)e^{i\omega_k 0^+}$, and $D_F = mk_F/\pi^2 (=3n/mv_F^2)$ is the density of states of the noninteracting system at its Fermi energy ϵ_F . If we put $\omega_q = 0$ in Eq. (11b), we find an exact result for $\Pi^{11}(\mathbf{q}, \omega_q)$ at $\omega_q = 0$ as

$$\Pi^{11}(\mathbf{q}, 0) = \frac{D_F}{3}. \quad (12)$$

In the interacting-electron system with translational symmetry, the total charge current (or the total momentum) is conserved; namely, $(\partial/\partial t) \int d^3r \mathbf{j}(\mathbf{r}, t) = 0$. This global velocity conservation law allows us to derive an identity for $\Gamma^1(K, K + Q)$ in the limit of $v_F q/\omega_q \rightarrow 0$ as

$$\frac{\Gamma^1(K, K + Q)}{\gamma^1(K, K + Q)} = \frac{G^{-1}(K + Q) - G^{-1}(K)}{i\omega_q} \left[1 + O\left(\frac{v_F q}{\omega_q}\right) \right]. \quad (13)$$

By substituting Eq. (13) into Eq. (7), we can easily find another exact result for $\Pi^{11}(\mathbf{q}, \omega_q)$ at $\mathbf{q} = \mathbf{0}$ as

$$\Pi^{11}(\mathbf{0}, \omega_q) = 0. \quad (14)$$

We can combine Eq. (13) with Eq. (10) to obtain an identity for $\Gamma^0(K, K + Q)$ in the limit of $v_F q/\omega_q \rightarrow 0$ as

$$\begin{aligned} \Gamma^0(K, K + Q) &= \frac{G^{-1}(K + Q) - G^{-1}(K)}{i\omega_q} \\ &\times \left[1 + \frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{i\omega_q} + O\left(\frac{v_F^2 q^2}{\omega_q^2}\right) \right]. \quad (15) \end{aligned}$$

By substituting the above equation into Eq. (7), we find an exact result for $\Pi^{00}(\mathbf{q}, \omega_q)$ as

$$\Pi^{00}(\mathbf{q}, \omega_q) = \frac{D_F q^2 v_F^2}{3 \omega_q^2} + O\left(\frac{v_F^3 q^3}{\omega_q^3}\right), \quad (16)$$

in the limit of $v_F q / \omega_q \rightarrow 0$. This behavior of $\Pi^{00}(\mathbf{q}, \omega_q)$ is known as the frequency sum rule.

At $q = \omega_q = 0$, Eq. (15) does not hold; it is replaced by

$$\Gamma^0(K, K) = \frac{\partial G^{-1}(K)}{\partial \mu}, \quad (17)$$

as one can convince oneself by considering the one-to-one correspondence of each Feynman diagram representing $\Gamma^0(K, K)$ with the one obtained by the differentiation of an arbitrary G line in each Feynman diagram for Σ with respect to μ . Then, by putting Eq. (17) into Eq. (7) and using $\partial G^{-1}(K) / \partial \mu = -G^{-1}(K) [\partial G(K) / \partial \mu] G^{-1}(K)$, we find another exact result for $\Pi^{00}(\mathbf{q}, \omega_q)$ at $q = \omega_q = 0$ as

$$\Pi^{00}(\mathbf{0}, 0) = \frac{dn}{d\mu}, \quad (18)$$

where the total electron number density n is given by $n = 2 \int d^3k n(\mathbf{k}) / (2\pi)^3$. The relation in Eq. (18) is known as the compressibility sum rule.

III. PERSPECTIVE FROM FERMI-LIQUID THEORY

A. Quasiparticles on and near the Fermi surface

In configuring a successful functional form for $\Gamma^0[\Sigma]$, we presume that the exact results in Eqs. (15) and (17) provide invaluable boundary conditions. Thus, with the aim of constructing a good interpolation formula for $\Gamma^0(K, K + Q)$ satisfying these two conditions exactly, we shall begin with revisiting the Fermi-liquid theory that is conventionally formulated at $T = 0$.

In order to extract the physical results from $G(K)$ obtained on the imaginary axis $i\omega_k$, we need to make its analytic continuation to the real axis on the upper- ω_k plane. Then, a pole of $G(K)$ on the lower- ω_k plane describes the excitation energy of a quasiparticle. For an isotropic system, $G(K)$ may be considered as a function of two variables, $\epsilon_{\mathbf{k}}$ and ω_k , i.e., $G(K) = G(\epsilon_{\mathbf{k}}, \omega_k)$, and its inverse vanishes on the Fermi surface as

$$G^{-1}(\epsilon_{\mathbf{k}} = \epsilon_F, \omega_k = 0) = 0, \quad (19)$$

where $\epsilon_F \equiv \epsilon_{\mathbf{k}_F}$ is the *free-electron* chemical potential at $T = 0$, which should be distinguished from the *interacting-electron* chemical potential μ . We can expand $G^{-1}(\epsilon_{\mathbf{k}}, \omega_k)$ with respect to $\epsilon_{\mathbf{k}} - \epsilon_F$ and ω_k as

$$G(K) = \frac{z}{i\omega_k - (m/m^*)(\epsilon_{\mathbf{k}} - \epsilon_F)} + \dots, \quad (20)$$

where the residue z and the effective mass m^* of the quasiparticle at the Fermi level are, respectively, related to the derivatives of $G^{-1}(\epsilon_{\mathbf{k}}, \omega_k)$ as

$$\left. \frac{\partial G^{-1}(K)}{\partial i\omega_k} \right|_{K=K_F} = \left. \frac{\partial G^{-1}(\epsilon_F, \omega_k)}{\partial i\omega_k} \right|_{\omega_k=0} = \frac{1}{z}, \quad (21a)$$

$$\left. \frac{\partial G^{-1}(K)}{\partial \epsilon_{\mathbf{k}}} \right|_{K=K_F} = \left. \frac{\partial G^{-1}(\epsilon_{\mathbf{k}}, 0)}{\partial \epsilon_{\mathbf{k}}} \right|_{\epsilon_{\mathbf{k}}=\epsilon_F} = -\frac{1}{z} \frac{m}{m^*}, \quad (21b)$$

with $K_F \equiv \{\mathbf{k}_F, \omega_k = 0\}$ denoting K at the Fermi level.

Incidentally, it should be noted that $G(K)$ depends not only on its arguments, $\epsilon_{\mathbf{k}}$ and ω_k , but also on ϵ_F . By the total differentiation of Eq. (19) with respect to ϵ_F , however, we find

that $\partial G^{-1}(K) / \partial \epsilon_F$ is actually equal to $-\partial G^{-1}(K) / \partial \epsilon_{\mathbf{k}}$ on the Fermi surface, leading us to another important relation as

$$\left. \frac{\partial G^{-1}(K)}{\partial \epsilon_F} \right|_{K=K_F} = \left. \frac{\partial G^{-1}(\epsilon_{\mathbf{k}}, 0)}{\partial \epsilon_F} \right|_{\epsilon_{\mathbf{k}}=\epsilon_F} = \frac{1}{z} \frac{m}{m^*}. \quad (22)$$

B. Reduction to the zero-temperature formalism

At first glance, it might be thought to be possible to obtain an integral equation to determine $\Gamma^v(K, K + Q)$ at $T = 0$ easily by just replacing the sum over $\omega_{k'}$ in Eq. (6) by an integral over $\omega_{k'}$ as

$$T \sum_{\omega_{k'}} \dots \longrightarrow \int_{-\infty}^{\infty} \frac{d\omega_{k'}}{2\pi} \dots, \quad (23)$$

but it is not always the case. In fact, Eq. (6) contains a product of two Green's functions, $G(K')G(K' + Q)$, each of which possesses a quasiparticle's pole. The two simple poles merge into a single second-order one of $G^2(K')$ at $q = \omega_q = 0$, providing an extra term of the derivative of the Fermi distribution function, which is reduced to a negative δ function at $T = 0$. Thus we should adopt the replacement scheme prescribed by

$$\begin{aligned} T \sum_{\omega_{k'}} \dots G^2(K') \\ \longrightarrow \int_{-\infty}^{\infty} \frac{d\omega_{k'}}{2\pi} \dots \left[G^2(K') - 2\pi z^2 \frac{m^*}{m} \delta(\epsilon_{\mathbf{k}'} - \epsilon_F) \delta(\omega_{k'}) \right], \end{aligned} \quad (24)$$

instead of Eq. (23). Note that the δ -function term in Eq. (24) corresponds to the anomalous term that was found by Kohn and Luttinger in their study of the ground-state energy of an interacting Fermi gas.²¹

For finite but small q and ω_q , we need to modify Eq. (24) a little bit further by changing the product of two Green's functions as

$$\begin{aligned} G(K')G(K' + Q) \longrightarrow G^2(K') - \delta \left(\frac{\epsilon_{\mathbf{k}'+\mathbf{q}} + \epsilon_{\mathbf{k}'}}{2} - \epsilon_F \right) \\ \times \delta(\omega_{k'}) \frac{2\pi z^2 (\epsilon_{\mathbf{k}'+\mathbf{q}} - \epsilon_{\mathbf{k}'})}{(m/m^*)(\epsilon_{\mathbf{k}'+\mathbf{q}} - \epsilon_{\mathbf{k}'}) - i\omega_q}, \end{aligned} \quad (25)$$

which reduces to the replacement scheme in Eq. (24) in the so-called q limit ($q \rightarrow 0$ with $\omega_q = 0$). Thus the three-point vertex function in this limit $\Gamma_q^v(K)$, appearing in Fermi-liquid theory, directly connects with $\Gamma^v(K, K)$, such as the one in Eq. (17), in the finite-temperature formalism.

On the other hand, Eq. (25) reduces to $G^2(K')$ in the so-called ω limit ($\omega_q \rightarrow 0$ with $q = 0$), indicating that the simple replacement scheme in Eq. (23) applies to Eq. (6) in obtaining the three-point vertex function in Fermi-liquid theory in this limit $\Gamma_\omega^v(K)$, which is determined by

$$\Gamma_\omega^v(K) = \gamma^v(K) + 2 \int \frac{d^4 K'}{(2\pi)^4} \tilde{I}(K, K') G^2(K') \Gamma_\omega^v(K'), \quad (26)$$

with the definitions of $\gamma^v(K) \equiv \gamma^v(K, K)$, $\tilde{I}(K, K') \equiv \tilde{I}(K, K; K', K')$, and $\int d^4 K' \equiv \int d\omega_{k'} \int d^3 k'$.

Now in Fermi-liquid theory, it is useful to treat the physical quantities as a function of ϵ_F rather than μ . In fact, because of $d\epsilon_F/d\mu = \kappa/\kappa_F$ with κ and κ_F being the interacting-electron compressibility and the free-electron one, respectively, we can easily transform the argument from μ into ϵ_F to obtain the identity for $\Gamma_q^0(K)$ as

$$\Gamma_q^0(K) = \frac{\partial G^{-1}(K)}{\partial \mu} = \frac{\partial G^{-1}(K)}{\partial \epsilon_F} \frac{\kappa}{\kappa_F}, \quad (27)$$

from Eq. (17).

Since our system has rotational symmetry, the three-point vertex functions behave in the ω and q limits as

$$\Gamma_\omega^v(K) = \eta_\omega^v(\epsilon_{\mathbf{k}}, \omega_k) \cos \nu \theta_{\mathbf{k}\mathbf{q}}, \quad (28)$$

$$\Gamma_q^v(K) = \eta_q^v(\epsilon_{\mathbf{k}}, \omega_k) \cos \nu \theta_{\mathbf{k}\mathbf{q}}, \quad (29)$$

where $\theta_{\mathbf{k}\mathbf{q}}$ denotes the angle between \mathbf{k} and \mathbf{q} . The functions $\eta_\omega^v(\epsilon_{\mathbf{k}}, \omega_k)$ and $\eta_q^v(\epsilon_{\mathbf{k}}, \omega_k)$ are given as

$$\eta_\omega^0(\epsilon_{\mathbf{k}}, \omega_k) = \frac{\partial G^{-1}(K)}{\partial i\omega_k}, \quad (30a)$$

$$\eta_q^0(\epsilon_{\mathbf{k}}, \omega_k) = \frac{\partial G^{-1}(K)}{\partial \epsilon_F} \frac{\kappa}{\kappa_F}, \quad (30b)$$

$$\eta_\omega^1(\epsilon_{\mathbf{k}}, \omega_k) = \frac{\partial G^{-1}(K)}{\partial i\omega_k} \frac{k}{k_F}, \quad (30c)$$

$$\eta_q^1(\epsilon_{\mathbf{k}}, \omega_k) = -\frac{\partial G^{-1}(K)}{\partial \epsilon_{\mathbf{k}}} \frac{k}{k_F}, \quad (30d)$$

with reference to the results in Sec. II C. On the Fermi surface, with use of the results in Sec. III A, these functions are reduced to

$$\eta_\omega^0(\epsilon_F, 0) = \frac{1}{z}, \quad (31a)$$

$$\eta_q^0(\epsilon_F, 0) = \frac{1}{z(m^*/m)} \frac{\kappa}{\kappa_F}, \quad (31b)$$

$$\eta_\omega^1(\epsilon_F, 0) = \frac{1}{z}, \quad (31c)$$

$$\eta_q^1(\epsilon_F, 0) = \frac{1}{z(m^*/m)}. \quad (31d)$$

We can also make a similar argument on the polarization function $\Pi^{\nu\nu'}(Q)$ in each limit; in the ω limit, $\Pi^{\nu\nu'}(Q) \rightarrow \Pi_\omega^{\nu\nu'}$ with $\Pi_\omega^{\nu\nu'} = 0$ from global charge and velocity conservation laws, while in the q limit, $\Pi^{\nu\nu'}(Q) \rightarrow \Pi_q^{\nu\nu'} \delta_{\nu,\nu'}$ with

$$\Pi_q^{00} = D_F \frac{\kappa}{\kappa_F}, \quad (32a)$$

$$\Pi_q^{11} = \frac{D_F}{3}. \quad (32b)$$

Employing the replacement scheme prescribed by Eq. (23) with Eq. (25), together with the relation of $v_F^* q \cos \theta_{\mathbf{k}\mathbf{q}} = (m/m^*)(\epsilon_{\mathbf{k}'+\mathbf{q}/2} - \epsilon_{\mathbf{k}'-\mathbf{q}/2})$ with $v_F^* \equiv k_F/m^*$ being the velocity of the quasiparticle, we can reduce Eq. (6) to the zero-temperature Bethe-Salpeter equation to determine the three-point vertex function $\Gamma^v(K; Q) \equiv \Gamma^v(K - Q/2, K + Q/2)$

for small q and ω_q as

$$\begin{aligned} \Gamma^v(K; Q) &= \Gamma_\omega^v(K) - 2 \int \frac{d^4 K'}{(2\pi)^4} \tilde{I}_\omega(K, K') \Gamma^v(K'; Q) \\ &\quad \times \frac{2\pi z^2 v_F^* q \cos \theta_{\mathbf{k}'\mathbf{q}}}{v_F^* q \cos \theta_{\mathbf{k}'\mathbf{q}} - i\omega_q} \frac{m^*}{m} \delta(\epsilon_{\mathbf{k}'} - \epsilon_F) \delta(\omega_{k'}), \end{aligned} \quad (33)$$

where $\tilde{I}_\omega(K, K')$ the four-point vertex function in the ω limit satisfies the following integral equation:

$$\begin{aligned} \tilde{I}_\omega(K, K') &= \tilde{I}(K, K') + 2 \int \frac{d^4 K''}{(2\pi)^4} \tilde{I}(K, K'') \\ &\quad \times G^2(K'') \tilde{I}_\omega(K'', K'). \end{aligned} \quad (34)$$

Similarly, we can reduce Eq. (7) to the equation to determine the polarization function $\Pi^{\nu\nu'}(Q)$ at $T = 0$ for small q and ω_q as

$$\begin{aligned} \Pi^{\nu\nu'}(Q) &= \Pi_\omega^{\nu\nu'} + 2 \int \frac{d^4 K}{(2\pi)^4} \Gamma_\omega^v(K) \Gamma^v(K; Q) \\ &\quad \times \frac{2\pi z^2 v_F^* q \cos \theta_{\mathbf{k}\mathbf{q}}}{v_F^* q \cos \theta_{\mathbf{k}\mathbf{q}} - i\omega_q} \frac{m^*}{m} \delta(\epsilon_{\mathbf{k}} - \epsilon_F) \delta(\omega_k), \end{aligned} \quad (35)$$

in which $\Pi_\omega^{\nu\nu'} = 0$ in our present system.

C. Spherical-harmonics expansion

The central quantity in Fermi-liquid theory is the Landau interaction $f(\mathbf{k}_F, \mathbf{k}'_F)$, which is defined on the Fermi surface as $f(\mathbf{k}_F, \mathbf{k}'_F) \equiv z^2 \tilde{I}_\omega(K_F, K'_F)$. This quantity is just enough for the proper description of $\Pi^{\nu\nu'}(Q)$, but we find it necessary to extend its definition so as to include the information on its momentum-frequency dependence for the adequate description of $\Gamma^v(K; Q)$.

The extension can be done straightforwardly by expanding $\tilde{I}_\omega(K, K')$ in terms of the spherical harmonics. More specifically, by virtue of the spherical symmetry of our system, it is expanded as

$$\tilde{I}_\omega(K, K') = \sum_{\ell=0}^{\infty} \tilde{I}_{\omega,\ell}(\epsilon_{\mathbf{k}}, \omega_k; \epsilon_{\mathbf{k}'}, \omega_{k'}) P_\ell(\cos \theta_{\mathbf{k}\mathbf{k}'}), \quad (36)$$

where $P_\ell(\cos \theta_{\mathbf{k}\mathbf{k}'})$ are the Legendre polynomials of $\cos \theta_{\mathbf{k}\mathbf{k}'}$ with $\theta_{\mathbf{k}\mathbf{k}'}$ being the angle between \mathbf{k} and \mathbf{k}' . A similar expansion can be made for the Landau interaction, and its ℓ 's component, $f_\ell(\epsilon_{\mathbf{k}}, \omega_k)$, may be defined as

$$f_\ell(\epsilon_{\mathbf{k}}, \omega_k) \equiv z^2 \tilde{I}_{\omega,\ell}(\epsilon_{\mathbf{k}}, \omega_k; \epsilon_F, 0). \quad (37)$$

Note that the standard Landau-interaction harmonics, f_ℓ , defined on the Fermi surface is given by $f_\ell = f_\ell(\epsilon_F, 0)$.

We can use this expansion to rewrite Eq. (35) as

$$\Pi^{\nu\nu'}(Q) = \Pi_\omega^{\nu\nu'} + z^2 \eta_\omega^v(\epsilon_F, 0) \Pi_{\nu\nu'}^*(Q) \eta_\omega^{\nu'}(\epsilon_F, 0), \quad (38)$$

for small q and ω_q , where $\Pi_{\ell\ell'}^*(Q)$ is the dynamical Fermi-surface susceptibility defined for arbitrary nonnegative integers $\ell, \ell' \geq 0$, the q limit of which quantifies the ‘‘softness’’ of a Fermi surface,^{22,23} and it is determined by

$$\Pi_{\ell\ell'}^*(Q) = \Pi_{\ell\ell'}^{*(0)}(Q) - \sum_{\ell''=0}^{\infty} \Pi_{\ell\ell''}^{*(0)}(Q) f_{\ell''} \Pi_{\ell''\ell'}^*(Q), \quad (39)$$

with

$$\Pi_{\ell\ell'}^{*(0)}(Q) \equiv \frac{D_F m^*}{2} \frac{1}{m} \int_{-1}^1 dx P_\ell(x) P_{\ell'}(x) \frac{v_F^* q x}{v_F^* q x - i\omega_q}. \quad (40)$$

Using Eqs. (31a) and (31c) and noting $\Pi_{\omega'}^{vv'} = 0$ in our system, we find $\Pi^{vv'}(Q) = \Pi_{vv'}^*(Q)$, but in general the following relation holds:

$$\frac{\Pi^{vv'}(Q) - \Pi_{\omega'}^{vv'}}{\Pi_{q, vv}^{vv} - \Pi_{\omega'}^{vv}} = \frac{\Pi_{vv'}^*(Q) \eta_{\omega'}^v(\epsilon_F, 0)}{\Pi_{q, vv}^* \eta_{\omega'}^v(\epsilon_F, 0)}, \quad (41)$$

where $\Pi_{q, vv}^* \equiv \Pi_{vv}^*(\mathbf{q}, \omega_q = 0)$ represents $\Pi_{vv}^*(Q)$ in the q limit. Because the velocity conservation law relates m^* to f_1 through $m^* = m/(1 - D_F f_1/3)$, Eq. (39) implies that $\Pi^{vv'}(Q)$ can be determined completely only by f_i 's.

Since our main interest is in $\Pi^{vv'}(Q)$ for $\omega_q/v_F^* q \ll 1$ and $\omega_q/v_F^* q \gg 1$, we shall neglect the contribution of f_i 's with $\ell \geq 2$ which becomes important only for $\omega_q/v_F^* q \sim 1$. Then we obtain

$$\Pi^{00}(Q) = \left[\frac{1}{\Pi_q^{00}} + \frac{1}{\Pi_q^{11}} \frac{\omega_q^2}{v_F^2 q^2} + \frac{c(|\omega_q|/v_F^* q) |\omega_q|}{\rho v_F q} \right]^{-1}, \quad (42a)$$

$$\Pi^{01}(Q) = \Pi^{10}(Q) = \frac{i\omega_q}{v_F q} \Pi^{00}(Q), \quad (42b)$$

$$\Pi^{11}(Q) = \Pi_q^{11} - \frac{\omega_q^2}{v_F^2 q^2} \Pi^{00}(Q), \quad (42c)$$

where $c(x)$ is a function defined by

$$c(x) \equiv \frac{\arctan(1/x)}{1 - x \arctan(1/x)} - 3x, \quad (43)$$

and it behaves as $c(x) = \pi/2 + O(x)$ for $x \ll 1$ and $c(x) = O(x^{-1})$ for $x \gg 1$. Thus we see that $\Pi^{vv'}(Q)$ depends weakly on m^*/m , if it does.

D. Functional form for vertex functions

We shall expand $\Gamma^v(K; Q)$ in a similar way as

$$\Gamma^v(K; Q) = \sum_{\ell=0}^{\infty} \Gamma_{\ell}^v(\epsilon_{\mathbf{k}}, \omega_k; Q) P_{\ell}(\cos \theta_{\mathbf{k}\mathbf{q}}), \quad (44)$$

and put this equation into Eq. (33), together with Eqs. (28) and (36), to obtain $\Gamma_{\ell}^v(\epsilon_{\mathbf{k}}, \omega_k; Q)$ for small q and ω_q as

$$\Gamma_{\ell}^v(\epsilon_{\mathbf{k}}, \omega_k; Q) = \delta_{\ell v} \eta_{\omega}^v(\epsilon_{\mathbf{k}}, \omega_k) - f_{\ell}(\epsilon_{\mathbf{k}}, \omega_k) \Pi_{\ell v}^*(Q) \eta_{\omega}^v(\epsilon_F, 0). \quad (45)$$

This clearly indicates that the knowledge of (not simply f_i 's but) $f_{\ell}(\epsilon_{\mathbf{k}}, \omega_k)$'s is needed to determine both scalar and longitudinal-vector vertex functions for small momentum-frequency transfer.

For the same reason as we mentioned in Sec. III C, we shall neglect $f_{\ell}(\epsilon_{\mathbf{k}}, \omega_k)$'s with $\ell \geq 2$ and try to derive useful formulas for the vertex functions that are asymptotically exact for both $\omega_q/v_F^* q \ll 1$ and $\omega_q/v_F^* q \gg 1$ with $q, \omega_q \rightarrow 0$. For this purpose, we first take the q limit in Eq. (45) to find

$$f_v(\epsilon_{\mathbf{k}}, \omega_k) = \frac{1}{\Pi_{q, vv}^*} \frac{\eta_{\omega}^v(\epsilon_{\mathbf{k}}, \omega_k) - \eta_q^v(\epsilon_{\mathbf{k}}, \omega_k)}{\eta_{\omega}^v(\epsilon_F, 0)}, \quad (46)$$

for $v = 0$ and 1. Notice that this constitutes an exact functional form for $f_v(\epsilon_{\mathbf{k}}, \omega_k)$. Substituting Eq. (46) back into Eq. (45) and using Eq. (41), we can derive

$$\Gamma_{v'}^v(\epsilon_{\mathbf{k}}, \omega_k; Q) = \delta_{v'v} \eta_{\omega}^v(\epsilon_{\mathbf{k}}, \omega_k) + [\eta_q^{v'}(\epsilon_{\mathbf{k}}, \omega_k) - \eta_{\omega}^{v'}(\epsilon_{\mathbf{k}}, \omega_k)] \times \frac{\Pi^{v'v}(Q) - \Pi_{\omega}^{v'v}}{\Pi_{q, v'v'}^{v'v} - \Pi_{\omega}^{v'v}}. \quad (47)$$

By neglecting the contributions with $\ell \geq 2$ in Eq. (44), we obtain

$$\Gamma^v(K; Q) = \eta_{\omega}^v(\epsilon_{\mathbf{k}}, \omega_k) \cos v \theta_{\mathbf{k}\mathbf{q}} + \sum_{v'=0}^1 [\eta_q^{v'}(\epsilon_{\mathbf{k}}, \omega_k) - \eta_{\omega}^{v'}(\epsilon_{\mathbf{k}}, \omega_k)] \times \frac{\Pi^{v'v}(Q) - \Pi_{\omega}^{v'v}}{\Pi_{q, v'v'}^{v'v} - \Pi_{\omega}^{v'v}} \cos v' \theta_{\mathbf{k}\mathbf{q}}. \quad (48)$$

The results in Eq. (48) provide general formulas for the scalar and longitudinal-vector vertex functions for small momentum-frequency transfer not only in 3D but also in 2D isotropic systems. It turns out that they also give exact formulas even for 1D systems except for $K = K_F$, if appropriate $\eta_{\omega}^v, \eta_q^v$, and $\Pi^{vv'}$ are used. (This will not be shown explicitly in this paper, but it will be elsewhere.)

In our system, all the quantities appearing on the right-hand side of Eq. (48) are already known in Eqs. (30), (32), and (42). Substituting those quantities into Eq. (48), we finally obtain asymptotically exact functional forms for the scalar and longitudinal-vector vertex functions, respectively, as

$$\Gamma^0(K; Q) = \frac{\partial G^{-1}(K)}{\partial i\omega_k} [1 - \bar{I}_{xc} \Pi^{00}(Q)] - \left[\frac{\partial G^{-1}(K)}{\partial i\omega_k} - \frac{\partial G^{-1}(K)}{\partial \epsilon_F} \right] \frac{1}{D_F} \Pi^{00}(Q) - \left[\frac{\partial G^{-1}(K)}{\partial i\omega_k} + \frac{\partial G^{-1}(K)}{\partial \epsilon_{\mathbf{k}}} \right] \times \frac{\epsilon_{\mathbf{k}+\mathbf{q}/2} - \epsilon_{\mathbf{k}-\mathbf{q}/2}}{D_F v_F q/3} \Pi^{10}(Q) \quad (49)$$

and

$$\Gamma^1(K; Q) = \frac{\partial G^{-1}(K)}{\partial i\omega_k} \left[\frac{\epsilon_{\mathbf{k}+\mathbf{q}/2} - \epsilon_{\mathbf{k}-\mathbf{q}/2}}{v_F q} - \bar{I}_{xc} \Pi^{01}(Q) \right] - \left[\frac{\partial G^{-1}(K)}{\partial i\omega_k} - \frac{\partial G^{-1}(K)}{\partial \epsilon_F} \right] \frac{1}{D_F} \Pi^{01}(Q) - \left[\frac{\partial G^{-1}(K)}{\partial i\omega_k} + \frac{\partial G^{-1}(K)}{\partial \epsilon_{\mathbf{k}}} \right] \times \frac{\epsilon_{\mathbf{k}+\mathbf{q}/2} - \epsilon_{\mathbf{k}-\mathbf{q}/2}}{D_F v_F q/3} \Pi^{11}(Q). \quad (50)$$

Here we have introduced $\bar{I}_{xc} \equiv D_F^{-1}(\kappa_F/\kappa - 1)$ for use in the next section.

IV. IMPROVED GWT SCHEME

A. Extrapolation with use of the ratio function

The result given in Eq. (49) for the scalar vertex function $\Gamma^0(K, K+Q)$ must be accurate for arbitrary incoming-electron momentum and frequency K as long as

the momentum-frequency transfer Q is small. But in order to obtain an accurate result for $\Sigma(K)$ through Eq. (9), we should know a good functional form for $\Gamma^0(K, K+Q)$ defined in the whole momentum-frequency space, necessitating an adequate extrapolation of $\Gamma^0(K, K+Q)$ from the small- Q region to the entire space. We can make such an extrapolation by exploiting the concept of “the ratio function” which was introduced in Ref. 8 to provide $\Gamma^0(K, K+Q)$ automatically satisfying the WI.

The ratio function $R(K, K+Q)$ is defined as

$$R(K, K+Q) \equiv \frac{\Gamma^0(K, K+Q) \gamma^1(K, K+Q)}{\Gamma^1(K, K+Q) \gamma^0(K, K+Q)}. \quad (51)$$

Combining this definition with Eq. (10), we obtain the exact expressions for $\Gamma^0(K, K+Q)$ and $\Gamma^1(K, K+Q)$ as

$$\Gamma^0(K, K+Q) = \frac{G^{-1}(K+Q) - G^{-1}(K)}{i\omega_q - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})/R(K, K+Q)}, \quad (52a)$$

$$\Gamma^1(K, K+Q) = \gamma^1(K, K+Q) \times \frac{G^{-1}(K+Q) - G^{-1}(K)}{i\omega_q R(K, K+Q) - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})}, \quad (52b)$$

respectively.

Now it is a very important point to note here that Eqs. (11a) and (11b) hold along with the WI in Eq. (10), if both $\Gamma^0(K, K+Q)$ and $\Gamma^1(K, K+Q)$ are determined at the same time through Eqs. (52a) and (52b) with use of the same form of $R(K, K+Q)$, whatever approximation is employed for $R(K, K+Q)$. Then, our strategy for providing a good extrapolation scheme for $\Gamma^0(K, K+Q)$ is to approximate $R(K, K+Q)$ in Eq. (51) by adopting Eqs. (49) and (50) for $\Gamma^0(K, K+Q)$ and $\Gamma^1(K, K+Q)$, respectively.

In the course of the adoption of those equations, we find it better to regard \bar{I}_{xc} as not just a constant but a function of some variables. Its actual function form is not known very well at this stage, but at least it must be a function of arbitrary values of q and ω_q as

$$\bar{I}_{xc} \longrightarrow \bar{I}_{xc}(Q) = \bar{I}_{xc}(q, \omega_q), \quad (53)$$

with the asymptotic behavior of $\bar{I}_{xc}(Q) \rightarrow D_F^{-1}(\kappa_F/\kappa - 1)$ in the q limit.

Since Γ^v and $\Pi^{vv'}$ are trivially related to Γ^0 and Π^{00} , respectively, through Eqs. (10), (11a), and (11b), we shall be concerned with only Γ^0 and Π^{00} hereafter and thus suppress their superscripts for simplicity; namely, $\Gamma(K, K+Q) \equiv \Gamma^0(K, K+Q)$ and $\Pi(Q) = \Pi(q, \omega_q) \equiv \Pi^{00}(Q)$.

In the present extrapolation scheme, the functional form for $\Gamma(K, K+Q)$ is cast into the product of two components as

$$\Gamma(K, K+Q) = \Gamma^{(a)}(K, K+Q) \Gamma^{(b)}(K, K+Q), \quad (54)$$

with

$$\Gamma^{(a)}(K, K+Q) = \frac{G^{-1}(K+Q) - G^{-1}(K)}{i\omega_q - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) \tilde{\eta}_1(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k)}, \quad (55a)$$

$$\Gamma^{(b)}(K, K+Q) = 1 - \bar{I}_{xc}(Q) \Pi(Q) - [1 - \tilde{\eta}_1(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k)] \times \frac{i\omega_q(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})}{v_F^2 q^2 / 3} \frac{1}{D_F} \Pi(Q) - [1 - \tilde{\eta}_2(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k)] \frac{1}{D_F} \Pi(Q), \quad (55b)$$

where the two new functions, $\tilde{\eta}_1(\epsilon_{\mathbf{k}}, \omega_k)$ and $\tilde{\eta}_2(\epsilon_{\mathbf{k}}, \omega_k)$, have been defined as

$$\tilde{\eta}_1(\epsilon_{\mathbf{k}}, \omega_k) \equiv - \frac{\partial G^{-1}(\epsilon_{\mathbf{k}}, \omega_k)}{\partial \epsilon_{\mathbf{k}}} \bigg/ \frac{\partial G^{-1}(\epsilon_{\mathbf{k}}, \omega_k)}{\partial i\omega_k}, \quad (56a)$$

$$\tilde{\eta}_2(\epsilon_{\mathbf{k}}, \omega_k) \equiv \frac{\partial G^{-1}(\epsilon_{\mathbf{k}}, \omega_k)}{\partial \epsilon_F} \bigg/ \frac{\partial G^{-1}(\epsilon_{\mathbf{k}}, \omega_k)}{\partial i\omega_k}. \quad (56b)$$

Simple manipulation after the substitution of Eq. (54) into Eq. (7) leads us to an expression to relate the function $\bar{I}_{xc}(Q)$ with the polarization function $\Pi(Q)$ as

$$\bar{I}_{xc}(Q) = \frac{1}{\Pi(Q)} - \frac{1}{\Phi_0(Q)} - \frac{1}{D_F} \left[1 + \frac{3\omega_q^2}{v_F^2 q^2} - \frac{3\omega_q^2}{v_F^2 q^2} \frac{\Phi_1(Q)}{\Phi_0(Q)} - \frac{\Phi_2(Q)}{\Phi_0(Q)} \right], \quad (57)$$

where the three “modified polarization functions” have been defined by

$$\Phi_0(Q) \equiv 2 \sum_K \frac{G(K+Q) - G(K)}{i\omega_q - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) \tilde{\eta}_1(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k)}, \quad (58a)$$

$$\Phi_1(Q) \equiv 2 \sum_K \frac{[G(K+Q) - G(K)](\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})}{[i\omega_q - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) \tilde{\eta}_1(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k)] i\omega_q}, \quad (58b)$$

$$\Phi_2(Q) \equiv 2 \sum_K \frac{[G(K+Q) - G(K)] \tilde{\eta}_2(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k)}{i\omega_q - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) \tilde{\eta}_1(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k)}. \quad (58c)$$

If we reduce these equations into those in the zero-temperature formalism by using the replacement scheme in Eq. (25), we can easily derive the asymptotic behavior at $q \rightarrow 0$ and $\omega_q \rightarrow 0$ for these polarization functions as

$$\Phi_0(Q) \rightarrow \tilde{\Phi}_0(x^*) \equiv z D_F \frac{m^*}{m} [1 - x^* \arctan(1/x^*)], \quad (59a)$$

$$\Phi_1(Q) \rightarrow \frac{m^*}{m} \tilde{\Phi}_0(x^*), \quad (59b)$$

$$\Phi_2(Q) \rightarrow (1-z) D_F + \frac{m}{m^*} \tilde{\Phi}_0(x^*), \quad (59c)$$

with $x^* \equiv |\omega_q|/(v_F^* q)$. By substituting Eqs. (42a) and (59a)–(59c) into Eq. (57), we can confirm that $\bar{I}_{xc}(Q) \rightarrow D_F^{-1}(\kappa_F/\kappa - 1)$ in the q limit.

Basically, the functions so far introduced in defining $\Gamma(K, K+Q)$ in Eq. (54) can actually be calculated, as long as $G(K)$ is provided. This means that this form of $\Gamma(K, K+Q)$ may be regarded as a functional of $G(K)$, or equivalently a functional of $\Sigma(K)$, by referring to the Dyson equation or Eq. (5), implying that we now have obtained the pursued improved functional form for $\Gamma[\Sigma]$ with which we can determine the self-consistent self-energy $\Sigma(K)$ in combination with Eqs. (7)–(9).

B. Connection with GISC and GWT schemes

The present framework with use of the functional form in Eq. (54) for $\Gamma[\Sigma]$ is general enough to contain each of the GISC and GWT schemes as its special situation, as we shall show in the following.

On the simple assumption of $\tilde{\eta}_1(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k) = 1$ in Eq. (55a) and $\Gamma^{(b)}(K, K + Q) = 1$ in Eq. (54), we obtain $\Gamma[\Sigma]$ as

$$\Gamma(K, K + Q) = \Gamma^{(a)}(K, K + Q) = \Gamma_{\text{WI}}(K, K + Q), \quad (60)$$

with

$$\Gamma_{\text{WI}}(K, K + Q) \equiv \frac{G^{-1}(K + Q) - G^{-1}(K)}{G^{(0)-1}(K + Q) - G^{(0)-1}(K)}, \quad (61)$$

where the free-electron Green's function $G^{(0)}(K)$ is given by

$$G^{(0)}(K) = \frac{1}{i\omega_k + \epsilon_F - \epsilon_{\mathbf{k}}}. \quad (62)$$

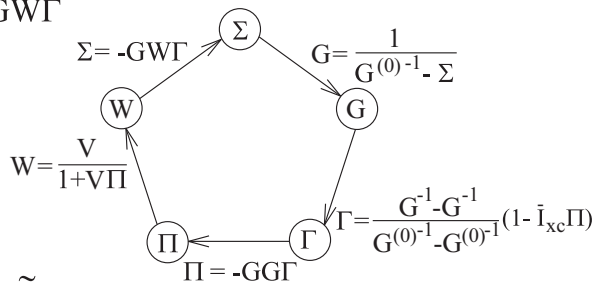
The GISC scheme¹² is proposed on the basis of this choice of $\Gamma[\Sigma]$ in Eq. (60) with Eq. (61). Although this seems to be a very simple scheme, it always satisfies the WI, because the choice of $R(K, K + Q) = 1$ in Eq. (52a) reproduces this form of $\Gamma[\Sigma]$ and for this reason, the subscript "WI" is attached to $\Gamma(K, K + Q)$ in Eq. (61). However, many other important sum rules including the compressibility one are not satisfied in this scheme.

If the assumption of $\tilde{\eta}_1(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k) = 1$ is retained but that of $\Gamma^{(b)}(K, K + Q) = 1$ is replaced by $\tilde{\eta}_2(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k) = 1$ in Eq. (55b), we obtain that $\Gamma^{(a)}(K, K + Q) = \Gamma_{\text{WI}}(K, K + Q)$ and $\Gamma^{(b)}(K, K + Q) = 1 - \tilde{I}_{\text{xc}}(Q)\Pi(Q)$. Thus $\Gamma[\Sigma]$ is provided by $\Gamma_{\text{WI}}(K + Q, K)[1 - \tilde{I}_{\text{xc}}(Q)\Pi(Q)]$, a result given in the $\text{GW}\Gamma$ scheme⁸ as schematically shown in Fig. 1(a).

In fact, on the assumption of both $\tilde{\eta}_1(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k)$ and $\tilde{\eta}_2(\epsilon_{\mathbf{k}+\mathbf{q}/2}, \omega_k)$ being unity, a further simplification can be made to this original $\text{GW}\Gamma$ scheme. First of all, all the modified polarization functions, $\Phi_0(Q)$, $\Phi_1(Q)$, and $\Phi_2(Q)$ in Eqs. (58a)–(58c), are reduced to the same single polarization function $\Pi_{\text{WI}}(Q)$, defined by

$$\Pi_{\text{WI}}(Q) \equiv -2 \sum_K G(K)G(K + Q)\Gamma_{\text{WI}}(K + Q, K). \quad (63)$$

(a) $\text{GW}\Gamma$



(b) $\text{G}\tilde{\text{W}}\Gamma_{\text{WI}}$

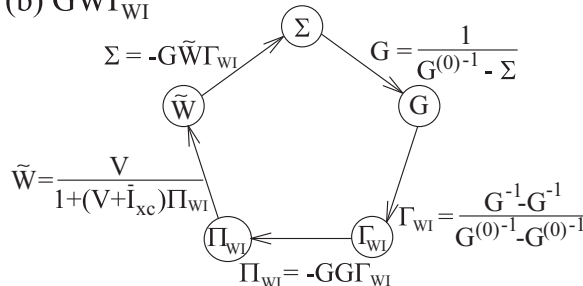


FIG. 1. Self-consistent iteration loops to determine the self-energy $\Sigma(K)$ in the $\text{GW}\Gamma$ scheme: (a) the original version and (b) the improved one, named the $\text{G}\tilde{\text{W}}\Gamma_{\text{WI}}$ scheme.

With use of $\Pi_{\text{WI}}(Q)$ and Eq. (57), we can represent the polarization function $\Pi(Q)$ as

$$\Pi(Q) = \frac{\Pi_{\text{WI}}(Q)}{1 + \tilde{I}_{\text{xc}}(Q)\Pi_{\text{WI}}(Q)}. \quad (64)$$

Then we can rewrite $\Sigma(K)$ in Eq. (9) into

$$\Sigma(K) = - \sum_Q \tilde{W}(Q) \Gamma_{\text{WI}}(K + Q, K) G(K + Q), \quad (65)$$

with $\tilde{W}(Q)$ the modified dynamically screened interaction, obtained from $W(Q)$ in Eq. (8) as

$$\tilde{W}(Q) \equiv \frac{V(\mathbf{q})}{1 + [V(\mathbf{q}) + \tilde{I}_{\text{xc}}(Q)]\Pi_{\text{WI}}(Q)}. \quad (66)$$

Combining these results, together with the Dyson equation, we can construct the $\text{G}\tilde{\text{W}}\Gamma_{\text{WI}}$ scheme as schematically shown in Fig. 1(b). This scheme is equivalent to the $\text{GW}\Gamma$ one in obtaining $\Sigma(K)$, but it is a merit that this is free from the problem of the dielectric catastrophe from which the original $\text{GW}\Gamma$ suffers, because the iteration loop in the $\text{G}\tilde{\text{W}}\Gamma_{\text{WI}}$ does not contain the process of calculating $\Pi(Q)$, a physical quantity which diverges at $r_s = 5.25$ in the electron gas.

A further merit in the $\text{G}\tilde{\text{W}}\Gamma_{\text{WI}}$ is a huge reduction of computational costs to calculate $\Pi(Q)$ not by Eq. (7) but by Eq. (64) via $\Pi_{\text{WI}}(Q)$ in Eq. (63) which can be cast into a form convenient for numerical calculations as

$$\Pi_{\text{WI}}(Q) = 2 \int \frac{d^3k}{(2\pi)^3} \frac{n(\mathbf{k} + \mathbf{q}) - n(\mathbf{k})}{i\omega_q - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}}, \quad (67)$$

with use of the interacting-electron momentum distribution function $n(\mathbf{k})$. Note that this expression very much resembles the one for the polarization function in the random-phase approximation (RPA) $\Pi^{(0)}(Q)$, which is given by

$$\Pi^{(0)}(Q) = 2 \int \frac{d^3k}{(2\pi)^3} \frac{n^{(0)}(\mathbf{k} + \mathbf{q}) - n^{(0)}(\mathbf{k})}{i\omega_q - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}}, \quad (68)$$

where $n^{(0)}(\mathbf{k}) [\equiv \theta(k_F - k)]$ is the free-electron momentum distribution function.

In spite of these merits of regarding Eq. (57) as an equation to determine not $\tilde{I}_{\text{xc}}(Q)$ but $\Pi(Q)$, we are now confronted with a serious problem of how to obtain $\tilde{I}_{\text{xc}}(Q)$. Actually, the problem may be traced back to the very assumption of $\tilde{\eta}_1 = \tilde{\eta}_2 = 1$ in which the result of $\Phi_0(Q) = \Phi_2(Q)$ clearly contradicts the asymptotic behaviors described in Eqs. (59a) and (59c), indicating that we should reconsider the asymptotic behavior of $\tilde{I}_{\text{xc}}(Q)$ itself in the q limit under this assumption.

In this circumstance, we shall take the strategy to provide a proper form of $\tilde{I}_{\text{xc}}(Q)$ by hand in the $\text{G}\tilde{\text{W}}\Gamma_{\text{WI}}$, rather than updating it automatically during the iteration process. In constructing the proper form for $\tilde{I}_{\text{xc}}(Q)$, we shall exploit the compressibility sum rule; in the q limit, $\Pi(\mathbf{0}, 0)$ is known as the value in Eq. (18), while $\Pi_{\text{WI}}(\mathbf{0}, 0)$ can be calculated from Eq. (67). Then we can determine $\tilde{I}_{\text{xc}}(\mathbf{0}, 0)$ through Eq. (64) with use of both $\Pi(\mathbf{0}, 0)$ and $\Pi_{\text{WI}}(\mathbf{0}, 0)$. In this way we can impose the compressibility sum rule exactly on the $\text{G}\tilde{\text{W}}\Gamma_{\text{WI}}$ scheme.

The difference between the GWA and this $\text{G}\tilde{\text{W}}\Gamma_{\text{WI}}$ in actual computational costs is not very large, mainly because the similarity between Eqs. (67) and (68) implies that the polarization function in each method can be obtained in an

analogous way. The only major difference lies in the existence of Γ_{WI} in Eq. (65), but this does not make the computational costs very much different.

In the $\tilde{\text{GW}}\Gamma_{\text{WI}}$, because the WI is obeyed, the electron number is conserved on the microscopic level and thus it is conserved on the macroscopic level as well. The conserving property of this scheme may also be assured by explicitly considering gauge invariance; because, as Baym discussed,⁵ G transforms in accord with $G^{(0)}$ with the change of gauge, Γ_{WI} is gauge-invariant, implying that the conserving property of Σ in the $\tilde{\text{GW}}\Gamma_{\text{WI}}$ is the same as that without Γ_{WI} , i.e., in the GWA. Since the GWA is a conserving approximation, the same is true for the $\tilde{\text{GW}}\Gamma_{\text{WI}}$.

C. Application to electron gas

Let us apply the improved $\text{GW}\Gamma$ method or the $\tilde{\text{GW}}\Gamma_{\text{WI}}$ scheme to the low-density electron gas in order to show that we can actually obtain $\Sigma(K)$ even for $r_s > 5.25$ in which κ becomes negative.

On general grounds, both $\tilde{\eta}_1$ and $\tilde{\eta}_2$ defined in Eqs. (56a) and (56b) are found to be equal to m/m^* on the Fermi surface due to the exact relations in Eqs. (30a)–(30d) and Eqs. (31a)–(31d). On the other hand, $G(K)$ approaches $G^{(0)}(K)$ far away from the Fermi surface, on which $\tilde{\eta}_1 \simeq \tilde{\eta}_2 \simeq 1$. Thus we may safely assume that both $\tilde{\eta}_1$ and $\tilde{\eta}_2$ vary in the range from m/m^* to 1.

Now in the electron-gas model at metallic densities, the effective mass m^* is known to be hardly different from the bare one m at least for r_s less than 6,^{3,24,25} implying that the approximation to take both $\tilde{\eta}_1$ and $\tilde{\eta}_2$ as unity, the basic assumption in deriving the $\tilde{\text{GW}}\Gamma_{\text{WI}}$ scheme, is expected to work very well in this model.

As for the choice of the proper form of $\tilde{I}_{\text{xc}}(Q)$, Eq. (64) reminds us of the long-standing research in the electron gas in pursuit of the appropriate local-field factor in the charge channel $G_+(Q)$. More specifically, we can expect that $\tilde{I}_{\text{xc}}(Q)$ must be equal to $-G_+(Q)V(\mathbf{q})$ with $G_+(Q)$ satisfying various sum rules such as the compressibility one. Note, however, that the meaning of $G_+(Q)$ here is different from the ordinary one that is defined with respect to $\Pi^{(0)}(Q)$ instead of $\Pi_{\text{WI}}(Q)$. Fortunately, we already know a good form for $G_+(Q)$ with taking account of this subtle difference, which is $G_s(Q)$ in Ref. 26, approaching the exact limit due to Niklasson²⁷ as $q \rightarrow \infty$ with $\omega_q = 0$.

With this choice of $\tilde{I}_{\text{xc}}(Q)$, the $\tilde{\text{GW}}\Gamma_{\text{WI}}$ provides us the self-consistent $\Sigma(K)$ in the electron gas for r_s going beyond 5.25, in spite of the existence of the dielectric catastrophe associated with negative κ . After analytic continuation ($i\omega_k \rightarrow \omega + i0^+$) of $\Sigma(K)$ to the retarded self-energy $\Sigma^R(\mathbf{k},\omega)$ with using the Padé approximant, we obtain the one-electron spectral function $A(\mathbf{k},\omega) [\equiv -\text{Im} G^R(\mathbf{k},\omega)/\pi]$; examples are plotted in Figs. 2(a)–2(c) at $k = 0$ (the center of the Fermi sphere), k_F (at the Fermi surface), and $1.4k_F$ (at which $\epsilon_{\mathbf{k}} - \epsilon_F = 0.96\epsilon_F \approx \epsilon_F$), respectively, for $r_s = 4, 5, 6$, and 8. The temperature is taken as $T = 0.001\epsilon_F$, virtually the same as zero temperature. The overall structure of $A(\mathbf{k},\omega)$ is shown in Figs. 3(a) and 3(b) as a function of ω for several values of k for $r_s = 4$ and 8, respectively, at $T = 0.001\epsilon_F$. Note that we have already seen a very similar structure of $A(\mathbf{k},\omega)$ at $r_s = 1$, which was given

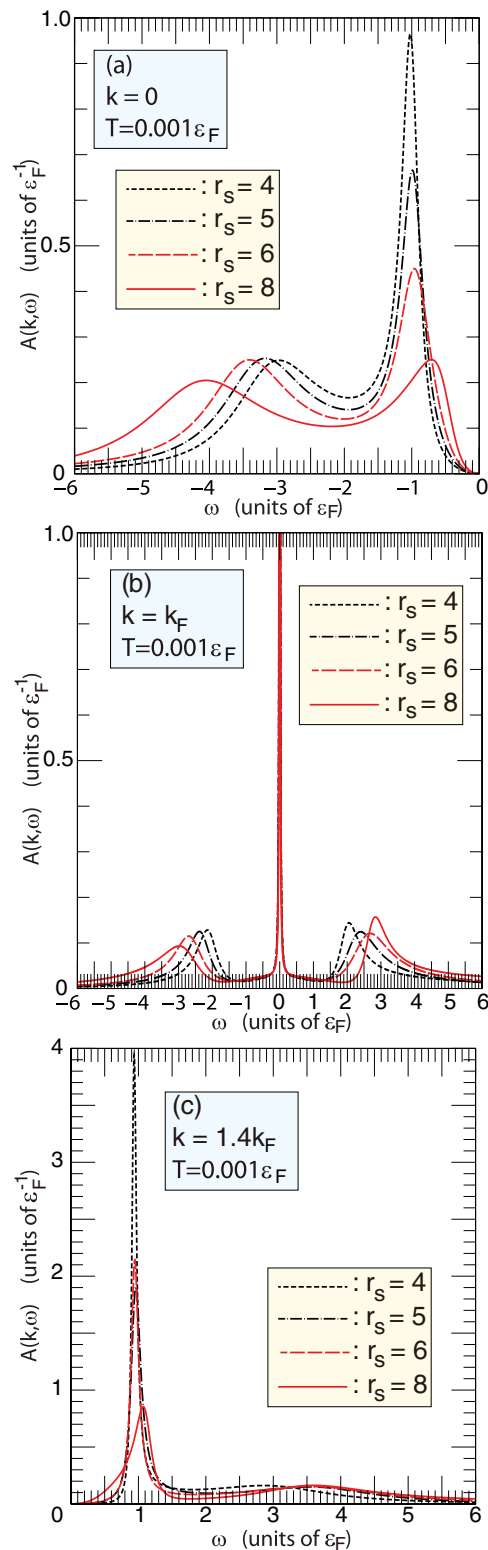


FIG. 2. (Color online) One-electron spectral function $A(\mathbf{k},\omega)$, plotted as a function of ω at (a) $k = 0$, (b) $k = k_F$, and (c) $k = 1.4k_F$ at $T = 0.001\epsilon_F$ in the electron gas for $r_s = 4, 5, 6$, and 8.

in Fig. 5 in Ref. 11 and might be considered as providing rather more typical Fermi-liquid behavior in the sense that the quasiparticles are very well defined for any values of k at $r_s = 1$.

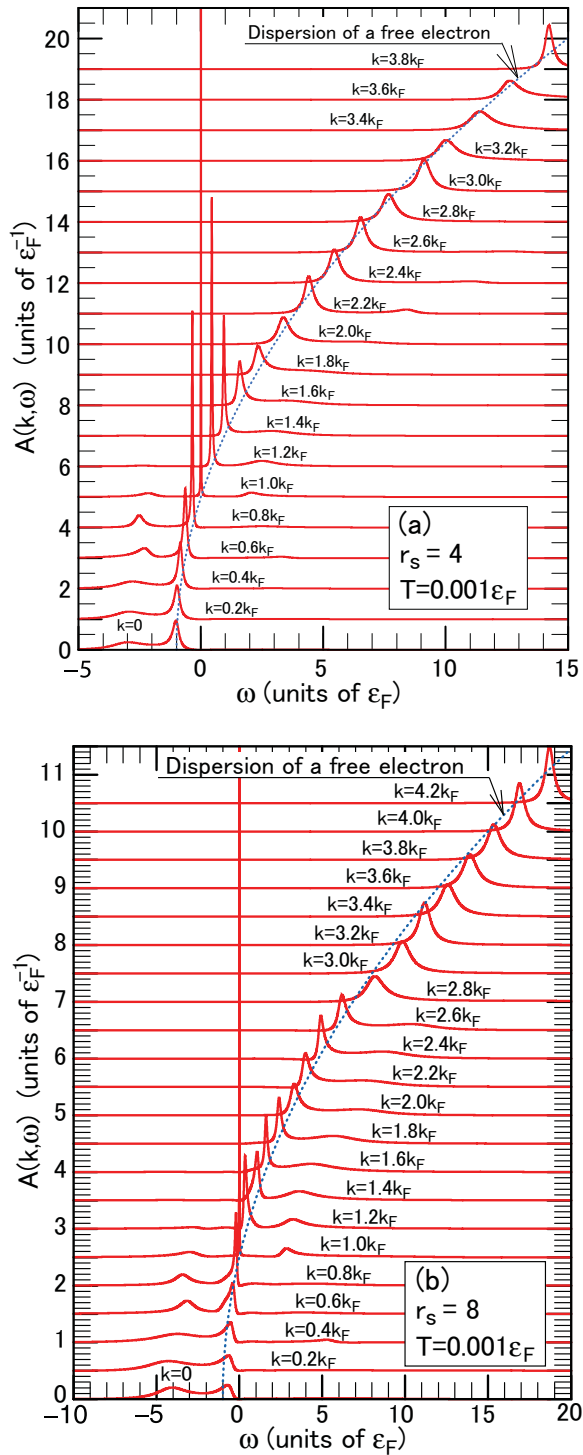


FIG. 3. (Color online) Overall structure of the one-electron spectral function $A(\mathbf{k}, \omega)$ in the electron gas at (a) $r_s = 4$ and (b) $r_s = 8$ with $T = 0.001 \epsilon_F$.

Several comments are in order on the results in Figs. 2 and 3:

(i) Although there is a difference in the choice of $\bar{I}_{xc}(Q)$, the present results for $k = 0$ and k_F at $r_s = 4$ are essentially the same as those given earlier in Fig. 2 in Ref. 8. In fact, we find that $A(\mathbf{k}, \omega)$ hardly depends on the choice of $\bar{I}_{xc}(Q)$, as long as the compressibility sum rule is satisfied.

(ii) The self-energy shift on the Fermi surface due to correlation depends rather sensitively on the choice of $\bar{I}_{xc}(Q)$, although this value itself does not show up at all in $A(\mathbf{k}, \omega)$, because it is canceled out by μ_c the contribution to the chemical potential from the correlation effect. We find that $G_s(Q)$ does not provide us an accurate enough value for μ_c , in spite of its very excellent features in obtaining other physical quantities,²⁸ prompting us to develop a better shape of $\bar{I}_{xc}(Q)$ in the near future.

(iii) An interesting result is found for the quasiparticle effective mass m^* at $r_s = 8$, in particular, for its k dependence; for k less than about $1.4k_F$, m^* is larger than m the free-electron mass, implying dominance of the correlation effect over the exchange one in determining m^* , while the opposite is the case for larger k to give $m^* < m$. This crossover in m^* in changing k never occurs for $r_s \lesssim 5$ where m^* is about the same as m ,^{8,29} as can be seen in Fig. 3(a) for $r_s = 4$, but it does occur for r_s larger than 5.25. Especially, the quasiparticle bandwidth shrinks by as large as 30% in the occupied portion at $r_s = 8$, but it does not in the unoccupied portion, as can be seen in Figs. 2(a) and 2(c). This feature in m^* is robust, even if we change the form of the compressibility-sum-rule conserving $\bar{I}_{xc}(Q)$ from the one in Ref. 26.

(iv) The very basic assumptions of $\bar{\eta}_1 = \bar{\eta}_2 = 1$ are justified for $r_s \lesssim 6$, because m^*/m is found to be around unity for any value of k , assuring us that the present results for $A(\mathbf{k}, \omega)$ must be very accurate. For the case of r_s as large as 8, however, the assumptions themselves are not well justified because of the large difference of m^* from m . Thus in the future, we will need to reformulate the GW Γ scheme without adopting those assumptions and examine to what extent the results of $A(\mathbf{k}, \omega)$ may deviate from the present ones in the revised scheme with including the effect of $m^*/m \neq 1$. In this regard, we do not consider that our present value of m^*/m at $r_s = 8$ is accurate enough, but even though such a revision is made, if we imagine how we can obtain a convergent result self-consistently with changing the value of m^*/m at each iteration step, we will probably end up with the qualitatively same crossover behavior of m^*/m with the increase of k .

(v) If k deviates from k_F , the quasiparticle peak in $A(\mathbf{k}, \omega)$ becomes broader as r_s becomes larger, for which it may be difficult to call a well-defined quasiparticle, but it is always well defined on the Fermi surface. Thus, as shown in Fig. 4, the momentum distribution function $n(\mathbf{k})$ exhibits a jump on the Fermi surface, a typical Fermi-liquid property, although its deviation from $n^{(0)}(\mathbf{k})$ becomes larger as r_s increases from $r_s = 2$, the typical density appropriate to most metals and semiconductors.

(vi) The magnitude of the jump as well as the overall structure of $n(\mathbf{k})$ in Fig. 4 agrees well with the accurate one,³⁰ if available, as already shown for $r_s = 4$ in Fig. 2(a) in Ref. 8. In fact, all of our present results for $n(\mathbf{k})$ satisfy the important sum rules of $\sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}^\ell n(\mathbf{k})$ for $\ell = 0$ (total number), $\ell = 1$ (kinetic energy),³⁰ and even $\ell = 2$ [fluctuation of kinetic energy or the sixth-order moment $\int dk k^6 n(\mathbf{k})$] at least up to six digits. It must be noted that those three sum rules will not be satisfied at the same time without quite accurate $n(\mathbf{k})$. Recently the reptation Monte Carlo (RMC) calculations have been done for $n(\mathbf{k})$ and their results are plotted in Fig. 4 for comparison.²⁰ A reasonably good agreement is seen for $r_s = 5$

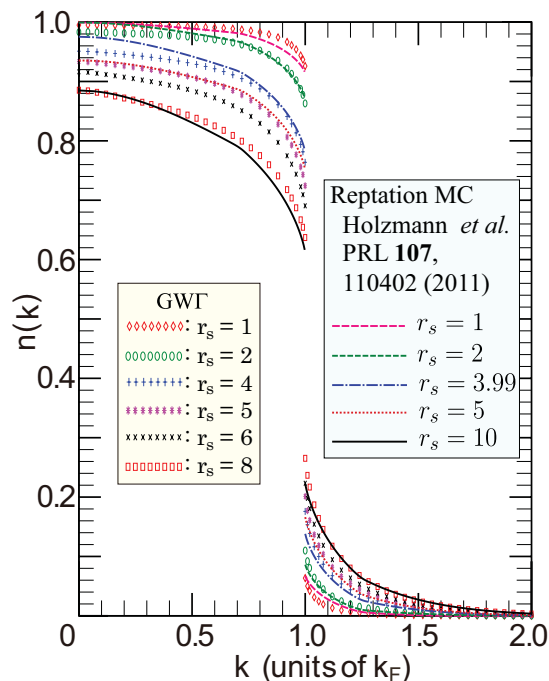


FIG. 4. (Color online) Momentum distribution function $n(\mathbf{k})$ for the electron gas at $r_s = 1$ (diamond), 2 (ellipse), 4 (plus), 5 (star), 6 (cross), and 8 (rectangle) in the GW method. For comparison, we also plot the recent results for $r_s = 1$ (longer dashed), 2 (dashed), 3.99 (dotted-dashed), 5 (dotted), and 10 (solid) in the reptation Monte Carlo method (Ref. 20).

in the entire region of k and for $r_s = 2$ and 4 in the region of k except for small values. A large discrepancy is seen for $r_s = 1$ and probably for $r_s = 10$ as well, although we have not yet obtained the result for $r_s = 10$, but our result for $r_s = 8$ almost agrees with the one for $r_s = 10$ in the RMC, clearly indicating that our result for $r_s = 10$ will be much different. Because of this discrepancy, the results of $n(\mathbf{k})$ in the RMC at least for $r_s = 10$ (and probably for all r_s except for $r_s = 5$) will hardly satisfy the important sum rules and thus they will not be so accurate, although no comments are made on the sum rules in Ref. 20. Upon careful examination of the RMC, we may think of at least the following three problems to make their results not so accurate: (1) the fixed-node approximation, (2) the extrapolation from data at $N = 54$ particles to those at $N \rightarrow \infty$, and (3) the use of the ideal-gas density matrix for reducing the variance. Probably the second point will be the reason for inaccuracy at $r_s = 1$ as well as in the small- k region for $r_s = 2$ and 4, while the third one will be at $r_s = 10$ at which the quasiparticle properties are much different from the noninteracting ones.

(vii) The results in the GWA as well as its one-shot version, the $G^{(0)}W^{(0)}A$, are not good enough in metals due to the neglect of the vertex corrections. The same is true in the electron gas in the description of not only the quasiparticle properties but also the peak position of the so-called plasmaron excitation, as already shown explicitly in Fig. 2(b) in Ref. 8 and in Fig. 4 in Ref. 11.

(viii) In clusters, insulators, and semiconductors at typical valence-electron densities (namely, $r_s \approx 2$), on the other hand,

we have already shown³¹ that the quasiparticle energies in the $G\tilde{W}\Gamma_{WI}$ are reasonably well described by the $G^{(0)}W^{(0)}A$.

V. ALTERNATIVE TO THE GW SCHEME

The basic strategy in the GW scheme is to regard $\tilde{I}_{xc}(Q)$ as an input quantity in view of the fact that its static function, $\tilde{I}_{xc}(\mathbf{q}, 0)$, is accurately known in the electron gas by the combination of Eq. (64) for $\Pi(Q)$ and the virtually exact data for the static polarization function $\Pi(\mathbf{q}, 0)$ obtained by diffusion Monte Carlo simulations.³²

In the general framework discussed in Sec. IV A, however, we do not necessarily require $\tilde{I}_{xc}(Q)$ as an input quantity but a quantity determined through Eq. (57), if $\Pi(Q)$ is accurately known beforehand. Now it is often the case in the many-body problem that $\Pi(Q)$ can be obtained much more easily than $G(K)$ by employing various theoretical techniques or even experimental data measured by either x-ray or neutron diffraction. In fact, $\Pi(Q)$ can be obtained from the first-principles Hamiltonian rather easily with use of the formalism due to Singwi, Tosi, Land, and Sjölander (STLS),³³ its recent refinement,³⁴ or its extension to the dynamical version.^{35–37} The same is true in the time-dependent density functional theory (TDDFT).^{38–40} Then we can think of an alternative to the GW scheme as shown schematically in Fig. 5. Because of the important role of $\tilde{I}_{xc}(Q)$ in this procedure, this may be called the $G\tilde{I}\Gamma$ scheme. Note that the dynamically screened interaction $W(Q)$ is known beforehand through Eq. (8) in this situation.

Based on the formally exact expression for $\Pi(Q)$ in the TDDFT, given by

$$\Pi(Q) = \frac{\Pi^{(0)}(Q)}{1 + f_{xc}(Q)\Pi^{(0)}(Q)}, \quad (69)$$

where $f_{xc}(Q)$ is the so-called exchange-correlation kernel, we only mention a very simplified version of this $G\tilde{I}\Gamma$ scheme here. Comparing Eq. (69) with Eq. (42a), we see that $f_{xc}(Q)$ is less singular than $\Pi^{(0)}(Q)$ and actually it is given by $f_{xc}(Q) = \tilde{I}_{xc}(q \rightarrow 0, \omega_q \rightarrow 0) = D_F^{-1}(\kappa_F/\kappa - 1)$ for small q and ω_q . On the other hand, by the Luttinger's theorem, Eq. (19), the chemical potential μ can be given in terms of the self-energy as $\mu = \epsilon_F + \Sigma(K_F)$, so that we see that

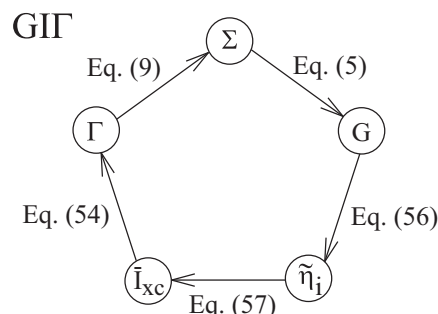


FIG. 5. Self-consistent iteration loop in the $G\tilde{I}\Gamma$ scheme to determine the self-energy $\Sigma(K)$ with use of the known information on $\Pi(Q)$.

$\kappa_F/\kappa = 1 + d\Sigma(K_F)/d\epsilon_F$. By combining these results, we can think of such a form for $f_{xc}(Q)$ as

$$f_{xc}^{\text{LDA}}(Q) = \frac{1}{D_F} \frac{d\Sigma(K_F)}{d\epsilon_F}, \quad (70)$$

in the local density approximation (LDA) in which its dependence on q and ω_q is totally neglected. Then we can give the polarization function in the LDA, $\Pi^{\text{LDA}}(Q)$, by adopting $f_{xc}^{\text{LDA}}(Q)$ evaluated through Eq. (70) with differentiating an input $\Sigma(K)$ as

$$\Pi^{\text{LDA}}(Q) = \frac{\Pi^{(0)}(Q)}{1 + f_{xc}^{\text{LDA}}(Q)\Pi^{(0)}(Q)}. \quad (71)$$

With use of this $\Pi^{\text{LDA}}(Q)$, we can follow the iteration loop in Fig. 5 to obtain the self-consistent self-energy $\Sigma(K)$. Note that $f_{xc}^{\text{LDA}}(Q)$ in this scheme depends on q and ω_q , although $f_{xc}^{\text{LDA}}(Q)$ does not. Note also that contrary to the original $\text{GI}\Gamma$ scheme, we do not require any information on $\Pi(Q)$ in the LDA, where $\Pi^{\text{LDA}}(Q)$ is revised in each iteration step to be determined from Eq. (71) self-consistently by virtue of Eq. (70). Of course, if an accurate value for κ_F/κ is known beforehand as is the case in the electron gas, we need not revise $f_{xc}^{\text{LDA}}(Q)$ at all, but instead we should maintain the relation of $f_{xc}^{\text{LDA}}(Q) = D_F^{-1}(\kappa_F/\kappa - 1)$ from the outset of the whole iteration process. The actual implementation along this procedure as well as the original $\text{GI}\Gamma$ scheme with use of a more accurate form for $\Pi(Q)$ is a challenge in the future.

VI. CONCLUSION

We have made a detailed analysis of the three-point vertex function Γ from the perspective of Fermi-liquid theory and constructed a functional form for Γ in Eq. (49) which should be accurate for small transferred momentum and frequency. The functional form is extrapolated to the one in the entire momentum-frequency space in Eqs. (55a) and (55b), the central result of this paper, which always satisfies the WI, along with other important sum rules. Based on this expression for Γ , we have discussed several versions of the self-consistent iteration procedure to determine the self-energy Σ , including the GISC, the original $\text{GW}\Gamma$, its improved version or the $\text{G}\tilde{\text{W}}\Gamma_{\text{WI}}$, and the $\text{GI}\Gamma$ schemes. In particular, the $\text{G}\tilde{\text{W}}\Gamma_{\text{WI}}$ scheme is employed to obtain Σ in the low-density electron gas

with use of the accurate information on the local-field factor for \tilde{I}_{xc} in Eq. (64), and the results for the one-electron spectral function $A(\mathbf{k}, \omega)$ and the momentum distribution function $n(\mathbf{k})$ are given in Figs. 2–4 for the density parameter r_s up to 8, elucidating the Fermi-liquid properties in a rather strongly correlated and dielectrically catastrophic region of the electron density. In future publications, we shall deal with the situations of 1D systems and systems without translational symmetry. We shall also investigate the electron gas at very low densities (i.e., $r_s \leq 10$) to obtain the accurate $n(\mathbf{k})$ for which the RMC will not seem to be a successful tool, as the results in Fig. 4 indicate.

All the calculation schemes proposed in this paper are based on the self-energy revision operator theory (SEROT) in which Σ is not calculated perturbatively, so that there is no problem of double counting. This problem of double counting hurts the usual perturbation methods including the so-called LDA + U and its refinements as well as the GWA + BS (Bethe-Salpeter) with use of the one-electron basis functions determined by the Kohn-Sham equation for which it is difficult to see to what extent the correlation effect is included from the outset of the perturbation calculation. Contrary to such a situation in the conventional perturbation theories, no problem of this kind arises in the SEROT. In fact, the only concern in it is to make a good approximate functional form for $\Gamma[\Sigma]$ to simulate the self-energy revision operator $\mathcal{F}[\Sigma_{\text{input}}]$ that is the operator to give the output self-energy $\Sigma_{\text{output}} (\equiv \mathcal{F}[\Sigma_{\text{input}}])$ by automatically adding new terms to the input self-energy Σ_{input} , indicating that the exact self-energy is obtained as the fixed point of \mathcal{F} , at which no new terms are added any more. For this very favorable feature, we believe that the SEROT provides the firm starting point for the numerical calculation of Σ in strongly correlated many-body systems in any spatial dimensions.

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