Improvement on the GWT Scheme for the Electron Self-Energy and Relevance of the $G_0W_0$ Approximation from this Perspective

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Based on an exact functional form derived for the three-point vertex function $\Gamma$, we propose a self-consistent calculation scheme for the electron self-energy with $\Gamma$ always satisfying the Ward identity. This scheme is basically equivalent to the one proposed in 2001, but it is improved in the aspects of computational costs and its applicability range; it can treat a low-density electron system with a dielectric catastrophe. If it is applied to semiconductors and insulators, we find that the obtained quasiparticle dispersion is virtually the same as that in the one-shot $GW$ approximation (or $G_0W_0A$), indicating that the $G_0W_0A$ actually takes proper account of both vertex and high-order self-energy corrections in a mutually cancelling manner.

KEYWORDS: self-energy, $GW$ approximation, vertex correction, Ward identity, self-consistency, insulator, semiconductor, quasiparticle, Fermi liquid, Tomonaga-Luttinger liquid

The electron self-energy $\Sigma$ is a fundamental quantity to control the quasiparticle properties in a many-electron system. Its accurate determination from first principles is recognized as a matter of central importance in many fields of condensed matter physics. In 1965, Hedin provided a nonperturbative self-consistent approach to $\Sigma$ in a closed set of equations, relating $\Sigma$ with the one-electron Green’s function $G$, the dynamic screened interaction $W$, the polarization function $\Pi$, and the vertex function $\Gamma$. In a closed set of equations, relating $\Sigma$ with the one-electron Green’s function $G$, the dynamic screened interaction $W$, the polarization function $\Pi$, and the vertex function $\Gamma$. This formally exact formulation, however, allows of no practical implementation in its original form, because we cannot calculate the electron-hole irreducible interaction $I$, a key quantity in the Bethe-Salpeter equation to determine $\Gamma$, through its original definition using a functional derivative, $I \equiv \delta \Sigma / \delta G$. Thus we are compelled to adopt some approximate treatments such as the $GW$ approximation (GWA) in which $\Gamma$ is taken as unity.

For more than two decades, successful calculations have been done for molecules, clusters, semiconductors, and insulators in the one-shot GWA (or $G_0W_0A$), but this is usually regarded as a too primitive approximation, mostly because it is, in general, not a conserving approximation in the sense of Baym and Kadanoff. In contrast, the GWA is a conserving one, obeying the conservation laws related to the macroscopic quantities like the total electron number. Upon implementation of this fully self-consistent GWA, however, we are led to a puzzling conclusion that the experiment on quasiparticle properties in semiconductors and insulators is much better described in the $G_0W_0A$ than in the GWA. A similar puzzle is also found in atoms and molecules.

In metals, on the other hand, neither the $G_0W_0A$ nor the GWA works very well, requiring us to include $\Gamma$ in some way in treating systems possessing gapless excitations. Some schemes have already been proposed for this purpose, but they do not satisfy the Ward identity (WI), an exact relation between $\Sigma$ and $\Gamma$ due to gauge invariance representing the local electron-number conservation. In 2001, based on general consideration on algorithms beyond the Baym-Kadanoff one, one of the authors (YT) proposed a scheme incorporating $\Gamma$ in the GWA with automatically fulfilling the WI. This GWT scheme (see, Fig. 1(a)) succeeded in obtaining the correct quasiparticle behavior in simple metals, but it encounters a serious difficulty in the low-density electron gas; convergent results for $\Sigma$ 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 $\kappa$ at $r_s = 5.25$ and concomitantly that of the static $\Pi$ in the long wave-length limit. Incidentally the GWA does not suffer from this difficulty, because $\Pi$ in it is not a physical one satisfying the compressibility sum rule.

In this Letter, we provide a new exact functional form for $\Gamma$, based on which we modify the GWT into a scheme free from the difficulty originating from the dielectric catastrophe. In order to illustrate the power of the modified scheme, which will be referred to as GWT$_W$ (see, Fig. 1(b)), we show the results calculated for the electron gas at $r_s = 8$. If it is applied to semiconductors and insulators, we find that the quasiparticle dispersion self-consistently obtained in the GWT$_W$ is essentially the same as that in the $G_0W_0A$, indicating that the $G_0W_0A$ is superior to the GWA in the sense that for the systems with gapful excitations, it actually takes proper account of the mutual cancellation between vertex and high-order self-energy corrections. This observation resolves the above-mentioned long-standing puzzle on the GWA in comparison with the $G_0W_0A$. Here we emphasize that this cancellation is proved to be the case up to infinite order in an analytically rigorous way with clarifying the assumptions needed in the proof, in sharp contrast with the claims of a similar kind in the past they were inferred from the behavior of low-order terms in perturbation expansion for metals.

Let us start with recapitulating the exact relations for...
systems with translation symmetry in which momentum \( \mathbf{p} \) is a good quantum number. The Dyson equation relates \( G(p) \) with \( \Sigma(p) \) through \( G(p)^{-1} = G_0(p)^{-1} - \Sigma(p) \) with \( p \) a combined notation of \( \mathbf{p} \), spin \( \sigma \), and fermion Matsubara frequency \( i \omega_n \equiv i \pi T (2n+1) \) at temperature \( T \) with an integer \( n \).\(^{24}\) The bare Green’s function \( G_0(p) \) is written as \( G_0(p) = \langle \omega_n - i \epsilon \rangle^{-1} \) with \( \epsilon_p \) the bare one-electron dispersion. The Bethe-Salpeter equation determines \( \Gamma(p, p+q) \) by

\[
\Gamma(p, p+q) = 1 + \sum_{p'} \bar{I}(p, p+q; p', p'+q) \\
\times G(p') G(p'+q) \Gamma(p', p'+q),
\]

(1)

where \( \sum_{p'} \) represents the sum \( T \sum_{\omega_n} \sum_{p'} \). With use of \( \Gamma(p, p+q) \), \( \Pi(q) \) and \( \Sigma(p) \) are, respectively, given by

\[
\Pi(q) = -\sum_p G(p) G(p+q) \Gamma(p, p+q),
\]

(2)

\[
\Sigma(p) = -\sum_q G(p+q) W(q) \Gamma(p, p+q),
\]

(3)

with \( W(q) = V(q)/[1 + V(q) \Pi(q)] \), where \( V(q) \) is the bare Coulomb interaction \( 4\pi\epsilon_0 q^2 \).

In Ref. 18, the concept of “the ratio function” was introduced to obtain an approximate functional form for \( \Gamma(p, p+q) \) satisfying the WI. By exploiting this concept, we have explored an exact functional form for \( \Gamma(p, p+q) \) and succeeded in obtaining the following form:

\[
\Gamma(p, p+q) = \Gamma^{(a)}(p, p+q) \Gamma^{(b)}(p, p+q),
\]

(4)

where \( \Gamma^{(a)}(p, p+q) \) and \( \Gamma^{(b)}(p, p+q) \) are, respectively, defined as \( \Gamma^{(a)}(p, p+q) \equiv 1 - \langle \bar{I} \rangle_{p, p+q} \Pi(q) \) and

\[
\Gamma^{(b)}(p, p+q) \equiv \frac{G(p+q)^{-1} - G(p)^{-1}}{G_0(p)^{-1} - G_0(p)^{-1} - \Delta \Sigma_{p, p+q}}.
\]

(5)

Here an average of \( \bar{I} \), \( \langle \bar{I} \rangle_{p, p+q} \), and a difference in the self-energy, \( \Delta \Sigma_{p, p+q} \), are, respectively, introduced by

\[
\langle \bar{I} \rangle_{p, p+q} = -\sum_{p'} \bar{I}(p, p+q; p', p'+q) \\
\times G(p') G(p'+q) \Gamma(p', p'+q)/\Pi(q),
\]

(6)

and

\[
\Delta \Sigma_{p, p+q} = \sum_{p'} \bar{I}(p, p+q; p', p'+q) [G(p'+q) - G(p')],
\]

(7)

as functionals of \( \bar{G} \) and \( \bar{I} \). If \( \bar{I} \) is exact, \( \Gamma^{(a)}(p, p+q) \) is nothing but \( \Gamma(p, p+q) \) in Eq. (1), as can easily be seen from the very definition of \( \langle \bar{I} \rangle_{p, p+q} \), and \( \Delta \Sigma_{p, p+q} \) is reduced to \( \Sigma(p+q) - \Sigma(p) \), leading to \( \Gamma^{(b)}(p, p+q) = 1 \). Thus Eq. (4) provides the same \( \Gamma(p, p+q) \) as that in the Hedin’s exact theory. In reality, the exact \( \bar{I} \) is not known and we have to employ some approximate \( \bar{I} \), in which an advantage of Eq. (4) over Eq. (1) becomes apparent; the former provides \( \Gamma(p, p+q) \) satisfying the WI irrespective of the choice of \( \bar{I} \), while the latter does not.

Physically \( \bar{I} \) takes care of exchange and correlation effects in \( \Gamma(p, p+q) \) and it is well known that this physics can be captured by the local-field factor for the homogeneous electron gas or by the Jastrow factor for inhomogeneous systems. In either way, these effects are well described in terms of a function depending only on the inter-electron distance, which justifies to assume that \( \bar{I}(p, p+q; p', p'+q) \) depends only on \( q \) to write \( \bar{I}(p, p+q; p', p'+q) \equiv I(q) \). If this assumption is adopted in our exact framework, we obtain \( I(q)_{p, p+q} = I(q) \) and \( \Delta \Sigma_{p, p+q} = 0 \). Then, by defining \( \Pi_{W I}(p, p+q) \) by

\[
\Pi_{W I}(p, p+q) = \frac{G(p+q)^{-1} - G(p)^{-1}}{G_0(p)^{-1} - G_0(p)^{-1}},
\]

(8)

we obtain \( \Gamma(p, p+q) = [1 - \bar{I}(q) \Pi(q)] \Gamma_{W I}(p, p+q) \), a result given in Ref. 18, leading to the GWT in Fig. 1(a).

By substituting this result of \( \Gamma(p, p+q) \) into Eq. (2), we find that \( \Pi(q) \) is written as

\[
\Pi(q) = \frac{\Pi_{W I}(q)}{1 + \bar{I}(q) \Pi_{W I}(q)}.
\]

(9)

with \( \Pi_{W I}(q) \), defined by

\[
\Pi_{W I}(q) = -\sum_p G(p) G(p+q) \Gamma_{W I}(p, p+q),
\]

(10)

Then we can rewrite \( \Sigma(p) \) in Eq. (3) into

\[
\Sigma(p) = -\sum_q G(p+q) \bar{W}(q) \Gamma_{W I}(p, p+q),
\]

(11)

with \( \bar{W}(q) \equiv V(q)/[1 + V(q) + \bar{I}(q)] \Pi_{W I}(q) \). Combining these results, we can construct the GWT WI scheme shown in Fig. 1(b). This scheme is equivalent to the GWT in obtaining \( \Sigma(p) \), but it is free from the problem of the dielectric catastrophe, because it does not contain the calculation of \( \Pi(q) \) inside the iteration loop.

It also renders a great advantage to the reduction of computational costs to calculate \( \Pi(q) \) not directly but by Eq. (9) via \( \Pi_{W I}(q) \), because Eq. (10) can be cast into a form convenient for numerical calculations as

\[
\Pi_{W I}(q) = \Pi_{W I}(q, i \omega_q) = \sum_{p \sigma} \frac{n(p+q) \delta(p)}{\omega_q - \epsilon_{p, p+q}^{\sigma} + \epsilon_p},
\]

(12)

where \( \omega_q \) is the boson Matsubara frequency and \( n(p) \equiv T \sum \mathrm{e}^{(p+q) e^{i \omega_q} + (p^0)} \) is the momentum distribution function. 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

\[
\Pi_0(q) = -\sum_p G_0(p) G_0(p+q) = \sum_{p \sigma} \frac{f(\epsilon_{p, p+q}^{\sigma}) - f(\epsilon_p^{\sigma})}{\omega_q - \epsilon_{p, p+q}^{\sigma} + \epsilon_p},
\]

(13)
where \( f(\epsilon) \) is the Fermi distribution function.

Two comments are in order: (i) Since it is conserved on the microscopic level in our scheme, the electron number is conserved on the macroscopic level as well. We can assure this conservation law by explicitly considering gauge invariance; because, as Baym discussed, \( G \) transforms in accord with \( G_0 \) with the change of gauge, \( \Gamma_W I \) is gauge-invariant, implying that the conserving property of \( \Sigma \) in the GW\( \Gamma_W I \) is the same as that without \( \Gamma_W I \), i.e., in the GWA. (ii) With use of Eq. (8) and the introduction of \( \tilde{A}_p(\epsilon) \equiv A_p(\epsilon) - \sum_q W(q)/i(\epsilon_q + \epsilon_p) \), our scheme provides an integral equation to determine \( G(p) \) through

\[
(i\omega_n - \epsilon_p)G(p) = 1 + \sum_q \frac{W(q)G(p+q)}{i\omega_q - \epsilon_{p+q} + \epsilon_p}.
\]

On the assumption of \( \tilde{I}(q) = 0 \), this equation coincides with the one for obtaining the asymptotically exact \( G(p) \) in a neutral Fermi system such as the one-dimensional Tomonaga-Luttinger model \(^{25}\) or higher-dimensional models with strong forward scatterings. \(^{26}\) This coincidence clearly demonstrates the intrinsically nonperturbative nature of our framework.

Basically \( \tilde{I}(q) \) is at our disposal; it can be determined either by perturbation expansion or by some nonperturbative approach, but Eq. (9) suggests us to choose \( \tilde{I}(q) = -G_+(q)V(q) \) with \( G_+(q) \) the local-field factor. 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 \( \Pi_W I(q) \). Fortunately, we already know a good form for \( G_+(q) \) with taking account of this subtle difference, which is \( G_+(q) \) in Ref. 27, satisfying the exact limit due to Niklasson\(^ {28} \) as \( |q| \to \infty \).

With this choice of \( \tilde{I}(q) \), the GW\( \Gamma_W I \) provides us the self-consistent \( \Sigma(p) \) in the electron gas for \( r_s > 5.25 \), in spite of the existence of the dielectric catastrophe associated with negative \( \kappa \). After analytic continuation \( i\omega_n \to \omega + \epsilon \) of \( \Sigma(p) \) to the retarded self-energy \( \Sigma_R(p, \omega) \) with using the Padé approach, we obtain the one-electron spectral function \( A(p, \omega) \equiv -\text{Im} \Sigma_R(p, \omega)/\pi \); an example is plotted in Fig. 2(a) of this section, for \( r_s = 8 \) and \( T = 0.001E_F \) with \( E_F \) the Fermi energy. The corresponding result for \( n(p) \) is given in Fig. 2(b), exhibiting a jump at the Fermi level, a typical Fermi-liquid property, though its deviation from \( n_0(p) \equiv \theta(\epsilon_F - |p|) \) the step function with \( \epsilon_F \) the Fermi momentum is much larger than that at \( r_s = 2 \), the typical density appropriate to many metals and semiconductors. We find an interesting result for the quasiparticle effective mass \( m^* \) at \( r_s = 8 \); for \( |p| < 1.4p_F \), \( m^* \) is larger than \( m_e \) the free-electron mass, implying dominance of the correlation effect over the exchange one, while the opposite is the case for \( |p| > 1.4p_F \) to give \( m^* < m_e \). This crossover in \( m^* \) never occurs for \( r_s \leq 5 \) where \( m^* \) is always smaller than \( m_e \). \(^ {18,29} \)

In the crystalline case, each quantity involved in the GW\( \Gamma_W I \) should be represented in the matrix form with respect to the reciprocal-lattice vectors \( \{ \mathbf{K} \} \). For example, \( G(p) \) is a matrix composed of the elements \( \{ G_{\mathbf{K}}(\mathbf{p}, i\omega_n) \} \) with \( \mathbf{p} \) a wave vector in the first Brillouin zone. For some quantities, we need to add the conversion factors transforming from the plane-wave basis to the Bloch-function one in considering the matrix elements; for example, \( \Pi_{0, \mathbf{K}}(q) \) is given as

\[
\Pi_{0, \mathbf{K}}(q) = \sum_{n'p} \frac{f(\epsilon_{p+q}) - f(\epsilon_{n'p})}{i\omega_q - \epsilon_{p+q} + \epsilon_p} \times [\langle p|e^{-i(q\cdot K)}|n'p+q\rangle \langle n'p+q|e^{i(q\cdot K')}|p\rangle].
\]

With this understanding, we have applied the GW\( \Gamma_W I \) to semiconductors and insulators possessing a gap in electronic excitation energies. Then, without detailed computations, the self-consistently determined quasiparticle energy \( E_p \) in our scheme is found to be well approximated by that in the \( G_0W_0\Lambda \), as we explain in the following.

Let us assume that \( \Pi_W I(q) = \Pi_0(q) \) and \( \tilde{I}(q) = 0 \) for the time being. Then, we may rewrite Eq. (11) as

\[
\Sigma(p) = -\sum_q \frac{W_0(q)}{G_0(p+q) - G_0(p)} + \lambda(p)G(p)^{-1},
\]

with \( W_0(q) \equiv V(q)/[1 + V(q)\Pi_0(q)] \) and \( \lambda(p) \) a dimensionless function, defined by

\[
\lambda(p) = \lambda(p, i\omega_n) = \sum_q \frac{G(p+q)W_0(q)}{i\omega_q - \epsilon_{p+q} + \epsilon_p}.
\]

The quasiparticle dispersion \( E_p \) is determined by \( G^R(p, E_p)^{-1} = 0 \), amounting to \( E_p = \epsilon_p + \Sigma^R(p, E_p) \), where we obtain the “on-shell” self-energy as

\[
\Sigma^R(p, E_p) = -\sum_q \frac{W_0(q)}{i\omega_q - \epsilon_{p+q} + \epsilon_p}.
\]

by analytic continuation of \( \Sigma(p) \) in Eq. (16). In deriving Eq. (18), we have paid due attention to the convergence
of $\lambda^R(p, E_p)$ in gapful systems. In fact, provided that
$\bar{I}(q) = 0$, $\epsilon_p$ and the integral in the right-hand side in
Eq. (14) are, respectively, reduced to $E_p$ and $\lambda(p)$, leading
to the behavior of $G^R(p, \omega)$ for $\omega$ near $E_p$ as

$$G^R(p, \omega) \approx \frac{1 + \lambda^R(p, E_p)}{\omega + i0^+ - E_p}. \quad (19)$$

For comparison, let us consider the self-energy in the
$G_0W_0A$, which is given by $\Sigma_0(p) = -\sum_q G_0(p+q)W_0(q)$. By
analytic continuation $i\omega_n \rightarrow \epsilon_p + i0^+$, we obtain

$$\Sigma^R_0(p, \epsilon_p) = -\sum_q \frac{W_0(q)}{i\omega_q - \epsilon_p + q + \epsilon_p} \frac{1}{2} \sum_q W_0(q, \epsilon_p + q - \epsilon_p)$$
$$\times \left[ \coth \frac{\epsilon_p + q - \epsilon_p}{2T} - \tanh \frac{\epsilon_p + q - \epsilon_p}{2T} \right]. \quad (20)$$

Because the transition $p+q \rightarrow p$ involved in Eq. (20)
is relevant only for the interband transition, $|\epsilon_p + q - \epsilon_p|$ is always larger than $E_p$, the energy gap. At low $T$, the
chemical potential $\mu$ lies at the center of the band gap,
indicating that $|\epsilon_{p+q}| \geq E_p/2$. These two facts allow us to
safely neglect the contribution from the second sum in
Eq. (20), as long as $T \ll E_p$. Thus we may write $E_p$ the
quasiparticle dispersion in the $G_0W_0A$ as

$$E_p^0 = \epsilon_p + \Sigma^R_0(p, \epsilon_p, \omega) \epsilon_p - \sum_q \frac{W_0(q)}{i\omega_q - \epsilon_p + q + \epsilon_p}, \quad (21)$$

leading us to conclude that $E_p^0 = E_p$. Note, however,
that the spectral weight $Z_p = \int [-1 - \partial \Sigma^R_0(p, \omega)/\partial \omega] |_{\omega = \epsilon_p}$ is different from $1 + \lambda^R(p, E_p)$.

In the literature, $E_p^0$ is sometimes evaluated as $E_p^0 = \epsilon_p + \sum R(p, \epsilon_p)$ and there is a controversy as to whether this $Z_p$ should be included or not. As previously discussed in detail, 23) we consider it better not to include $Z_p$ so that the vertex corrections beyond the RPA are properly included, together with higher-order self-energy terms in a mutually cancelling manner. In fact, our present result of $E_p^0 = E_p$ without this factor $Z_p$ indicates that this feature of mutual cancellation reaches far up to infinite order in semiconductors and insulators.

Finally we comment on the two assumptions: (i) The difference between $\Pi_{W.I}$ and $\Pi_0$ arises only from that between $n(p)$ and $n_0(p)$. In usual semiconductors and insulators, the valence-electron density is high; for example, $n_{\text{Si}} = 2$ for Si. Now $n(p)$ in a metal at such $n_{\text{Si}}$ does not deviate much from $n_0(p)$ except for the states near the Fermi level, as shown in Fig. 2(b), but those states are absent from the outset in these gapful systems. Thus $n(p)$ is close to $n_0(p)$, leading to $\Pi_{W.I} \approx \Pi_0$. (ii) Justification of $\bar{I}$ = 0 has already been done by numerical studies in Ref. 3, in which $\bar{I}$ in our scheme is critically assessed in terms of $K_{xc}$ the density-derivative of the Kohn-Sham exchange-correlation potential. From an analytic point of view, it is enough to note that the basic processes to contribute to $\bar{I}$ are related to the interband electron-hole interactions, in which $|q|$ for principal processes is of the order of $|K|$, making $V(q)$ very small and $G_0(q)$ reach its asymptotic constant. Thus the effect of $\bar{I}$ is weak in semiconductors and insulators.

In summary, we have proposed the $\text{GW}_{W.I}$ scheme

for the fully self-consistent and conserving calculation of the
electron self-energy. This can be applied not only to metals in a wide range of densities but also to semiconductors and insulators, in which the obtained quasiparticle dispersion is close to that in the $G_0W_0A$, explaining, from a fundamental viewpoint of many-body physics, the reason why the $G_0W_0A$ better describes the experiment than the GWA in those gapful systems. We also realize that the role of $\bar{I}$, representing short-range exchange and correlation effects, is very much different between gapless and gapful systems; in the former, it can never be ignored to obtain the reliable quasiparticle behavior, but in the latter, it can be neglected, as long as the $G_0W_0A$ well reproduces the experiment. In this respect we can suggest that the $G_0W_0A$ should be performed with judiciously choosing the basis functions to make $\bar{I}$ and the difference between $\Pi_{W.I}$ and $\Pi_0$ as small as possible.

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