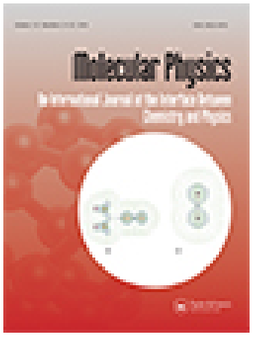

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# Role of the ward identity and relevance of the $G_0W_0$ approximation in normal and superconducting states

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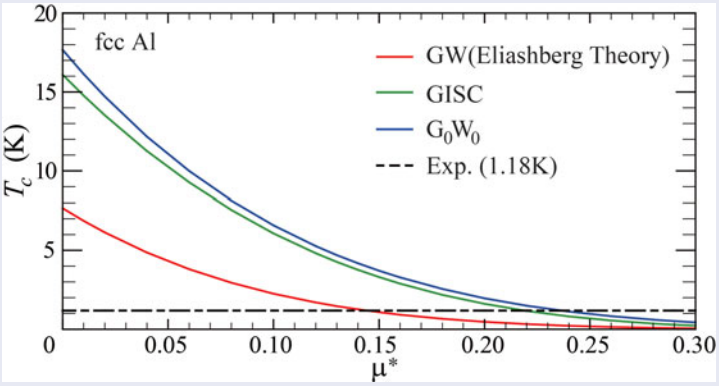
**ABSTRACT**

On the basis of the self-consistent calculation scheme for the electron self-energy $\Sigma$ with the use of the three-point vertex function $\Gamma$ always satisfying the Ward identity, we find that the obtained quasi-particle dispersion in the normal state in gapped systems, such as semiconductors, insulators, and molecules, is well reproduced by that in the one-shot GW (or $G_0W_0$) approximation. In calculating the superconducting transition temperature $T_c$, we also find a similar situation; the result for $T_c$ in the gauge-invariant self-consistent framework including the effect of $\Gamma$ satisfying the Ward identity is different from that in the conventional Eliashberg theory (which amounts to the GW approximation for superconductivity) but is close to that in the $G_0W_0$ approximation. Those facts indicate that the $G_0W_0$ approximation actually takes proper account of both vertex and high-order self-energy corrections in a mutually cancelling manner and thus we can understand that the $G_0W_0$ approximation is better than the fully self-consistent GW one in obtaining some of physical quantities.

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Superconductivity; vertex correction; ward identity; *GW* approximation; Eliashberg theory; gauge-invariant self-consistent (GISC) theory

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## 1. Introduction

A non-perturbative self-consistent approach to the electron self-energy $\Sigma$ was provided in 1965 by Hedin [1] in a closed set of equations, relating $\Sigma$ with the one-electron Green's function $G$, the dynamic screened interaction $W$, the polarisation function $\Pi$ and the vertex function $\Gamma$. This is a formally exact formulation, but it is difficult to implement this scheme as it is, because we cannot determine the electron–hole irreducible interaction $\tilde{I}$, a central quantity in the Bethe–Salpeter equation to calculate $\Gamma$, through its original definition using a functional derivative, $\tilde{I} = \delta\Sigma/\delta G$. Thus we are forced to adopt some approximate treatments such as the GW approximation 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 GW (or $G_0W_0$) approximation [2–7], 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 [8,9]. In contrast, the fully self-consistent GW approximation obeys the conservation laws related to the macroscopic quantities like the total electron number. In recent years, this self-consistent calculation has become feasible, but we are led to a puzzling conclusion that the experiment on quasi-particle properties in semiconductors and insulators is much better described in the $G_0W_0$ approximation than in the GW one [10,11]. In atoms and

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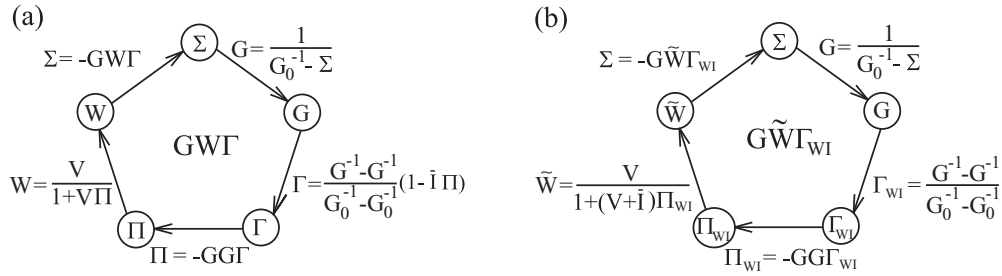


**Figure 1.** Self-consistent iteration loops to determine the electron self-energy (a) in the original GWΓ and (b) in its improved version or the $G\tilde{W}\Gamma_{WI}$, respectively.

molecules, the situation is less clear, but in many cases the $G_0W_0$ approximation gives better results [12–15].

In metals, on the other hand, neither $G_0W_0$ nor GW works very well [16], requiring us to include Γ in some way in treating systems possessing gapless excitations. Some schemes have already been proposed for this purpose [17,18], but they do not satisfy the Ward identity (WI), an exact relation between Σ and Γ due to gauge invariance representing the local electron-number conservation [19]. In 2001, based on general consideration on algorithms beyond the Baym–Kadanoff one [20], a scheme was proposed to incorporate Γ in the GW approximation with automatically fulfilling the WI [21]. This GWΓ scheme with the use of the information on the local-field factor in the electron gas [22] for determining $\tilde{I}$ (see Figure 1(a)) succeeded in obtaining the correct quasi-particle behaviour in simple metals. In 2011, this scheme was further improved [23] into the $G\tilde{W}\Gamma_{WI}$ scheme (see Figure 1(b)) so as to avoid the problem of dielectric catastrophe associated with the divergence of the compressibility $\kappa$ at the electron density specified by $r_s$ equal to 5.25 in the electron gas and concomitantly that of the static Π in the long wavelength limit [24,25]. This scheme is numerically confirmed to provide non-negative one-electron spectral functions $A(\boldsymbol{p}, \omega)$ for the homogeneous electron gas at least for $r_s \leq 8$ without any special treatments to impose on the positivity of $A(\boldsymbol{p}, \omega)$, contrary to a recently proposed scheme [26].

In the former part of this paper, we study the quasi-particle properties in the normal state to find that the quasi-particle dispersion self-consistently obtained in the $G\tilde{W}\Gamma_{WI}$ scheme for semiconductors and insulators is essentially the same as that in the $G_0W_0$ approximation, implying that $G_0W_0$ is superior to GW 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 GW versus $G_0W_0$. Here we emphasise that this cancellation is considered up to infinite order as a whole with specifying the assumptions needed in the cancellation, in sharp contrast with the claims of a similar kind in the past [27–29]; they were inferred from the behaviour of low-order terms in perturbation expansion for metals.

In the latter part of this paper, we study a similar problem in the superconducting state by the calculation of its transition temperature $T_c$ in the phonon mechanism in both the conventional Eliashberg theory [30–34] and the gauge-invariant self-consistent (GISC) method [35,36] which correspond, respectively, to the GW and GWΓ schemes for calculating the normal-state properties. Even for the case of weakly correlated and weakly coupled superconductors such as Al, we find that the calculated $T_c$ in GISC is different from that in the Eliashberg theory, but close to that in the $G_0W_0$ approximation. We discuss the implication of this result from various aspects, including the importance of determining the Coulomb pseudopotential $\mu^*$ [37] from first principles and a proposal of the suitable functional form for the pairing interaction kernel in the density functional theory for superconductors (SCDFT) [38–41].

## 2. Normal state

For systems with translation symmetry in which momentum $\boldsymbol{p}$ is a good quantum number, the exact Hedin's relations can be explicitly written in the following way: 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 $\boldsymbol{p}$, spin $\sigma$ and fermion Matsubara frequency $i\omega_p \equiv i\pi T(2p+1)$ at temperature $T$ with an integer $p$ [42]. The bare Green's function $G_0(p)$ is written as $G_0(p) = (i\omega_p - \varepsilon_{\boldsymbol{p}})^{-1}$ with $\varepsilon_{\boldsymbol{p}}$ the bare one-electron dispersion. The Bethe–Salpeter equation determines $\Gamma(p+q, p)$ by

$$\Gamma(p+q, p) = 1 + \sum_{p'} \tilde{I}(p+q, p; p'+q, p') G(p') \times G(p'+q)\Gamma(p'+q, p'), \quad (1)$$

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where $q$ is a combined notation of $\boldsymbol{q}$ and boson Matsubara frequency $i\omega_q \equiv i2\pi Tq$ with $q$ an integer and $\sum_{p'}$ represents the sum $T\sum_{\omega_{p'}}\sum_{\boldsymbol{p}'}\sum_{\sigma'}$. By using $\Gamma(p+q, p)$, we can give $\Pi(q)$ and $\Sigma(p)$ by

$$\Pi(q) = -\sum_{p} G(p+q)G(p)\Gamma(p+q, p), \tag{2}$$

$$\Sigma(p) = -\sum_{q} G(p+q)W(q)\Gamma(p+q, p), \tag{3}$$

respectively, with $\sum_q = T\sum_{\omega_q}\sum_{\boldsymbol{q}}$ and $W(q) = V(\boldsymbol{q})/[1+V(\boldsymbol{q})\Pi(q)]$, where $V(\boldsymbol{q})$ is the bare Coulomb interaction $4\pi e^2/\boldsymbol{q}^2$.

In [21], the concept of 'the ratio function' was introduced to obtain a good *approximate* functional form for $\Gamma(p+q, p)$ satisfying the WI. By exploiting this concept, we have explored an *exact* functional form for $\Gamma(p+q, p)$ and succeeded in obtaining the following form:

$$\Gamma(p+q, p) = \Gamma^{(a)}(p+q, p)\Gamma^{(b)}(p+q, p), \tag{4}$$

where $\Gamma^{(a)}(p+q, p)$ and $\Gamma^{(b)}(p+q, p)$ are, respectively, defined as

$$\Gamma^{(a)}(p+q, p) \equiv 1 - \langle\tilde{I}\rangle_{p+q,p}\Pi(q), \tag{5}$$

$$\Gamma^{(b)}(p+q, p) \equiv \frac{G(p+q)^{-1} - G(p)^{-1}}{G_0(p+q)^{-1} - G_0(p)^{-1} - \Delta\Sigma_{p+q,p}}. \tag{6}$$

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

$$\langle\tilde{I}\rangle_{p+q,p} \equiv -\sum_{p'}\tilde{I}(p+q, p; p'+q, p') \times G(p')G(p'+q)\Gamma(p'+q, p')/\Pi(q), \tag{7}$$

$$\Delta\Sigma_{p+q,p} \equiv \sum_{p'}\tilde{I}(p+q, p; p'+q, p')[G(p')-G(p'+q)], \tag{8}$$

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

Physically $\tilde{I}$ takes care of exchange and correlation effects in $\Gamma(p+q, p)$ 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 $\tilde{I}(p+q, p; p'+q, p')$ depends only on $q$ to write $\tilde{I}(p+q, p; p'+q, p') = \bar{I}(q)$. If this assumption is adopted in our exact framework, we obtain $\langle\tilde{I}\rangle_{p+q,p} = \bar{I}(q)$ and $\Delta\Sigma_{p+q,p} = 0$. Then, by defining $\Gamma_{WI}(p+q, p)$ by

$$\Gamma_{\rm WI}(p+q, p) \equiv \frac{G(p+q)^{-1} - G(p)^{-1}}{G_0(p+q)^{-1} - G_0(p)^{-1}}, \tag{9}$$

we obtain $\Gamma(p+q, p) = [1 - \bar{I}(q)\Pi(q)]\Gamma_{\rm WI}(p+q, p)$, a result given in [21], leading to the GW$\Gamma$ scheme in Figure 1(a).

By putting this form of $\Gamma(p+q, p)$ into Equation (2), we find that $\Pi(q)$ is written as

$$\Pi(q) = \frac{\Pi_{\rm WI}(q)}{1 + \bar{I}(q)\Pi_{\rm WI}(q)}, \tag{10}$$

with $\Pi_{WI}(q)$, defined by

$$\Pi_{\rm WI}(q) = -\sum_{p} G(p+q)G(p)\Gamma_{\rm WI}(p+q, p). \tag{11}$$

Then, we can rewrite $\Sigma(p)$ in Equation (3) into

$$\Sigma(p) = -\sum_{q} G(p+q)\tilde{W}(q)\Gamma_{\rm WI}(p+q, p), \tag{12}$$

with $\tilde{W}(q) \equiv V(\boldsymbol{q})/\{1 + [V(\boldsymbol{q}) + \bar{I}(q)]\Pi_{\rm WI}(q)\}$. Combining these results, we can construct the G$\tilde{\rm W}\Gamma_{\rm WI}$ scheme as shown in Figure 1(b). This scheme is equivalent to the GW$\Gamma$ one in obtaining $\Sigma(p)$, but computational costs are much reduced by the calculation of $\Pi(q)$ through Equation (10) via $\Pi_{WI}(q)$, because Equation (11) can be cast into a form convenient for numerical calculations as

$$\Pi_{\rm WI}(q) \equiv \Pi_{\rm WI}(\boldsymbol{q}, i\omega_q) = \sum_{\boldsymbol{p}\sigma}\frac{n(\boldsymbol{p}+\boldsymbol{q}) - n(\boldsymbol{p})}{i\omega_q - \varepsilon_{\boldsymbol{p}+\boldsymbol{q}} + \varepsilon_{\boldsymbol{p}}}, \tag{13}$$

where $n(\boldsymbol{p})$ [$= T\sum_{\omega_p} G(p)e^{i\omega_p 0^+}$] is the momentum distribution function in the interacting system. Note that this expression very much resembles the one for the

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polarisation function in the random-phase approximation (RPA) $\Pi_0(q)$, which is given by

$$\Pi_0(q) = -\sum_p G_0(p)G_0(p+q) = \sum_{\boldsymbol{p}\sigma} \frac{f(\varepsilon_{\boldsymbol{p}+\boldsymbol{q}}) - f(\varepsilon_{\boldsymbol{p}})}{i\omega_q - \varepsilon_{\boldsymbol{p}+\boldsymbol{q}} + \varepsilon_{\boldsymbol{p}}}, \tag{14}$$

where $f(\varepsilon)$ is the Fermi distribution function or the momentum distribution function in the non-interacting system.

With the use of Equation (9) and introducing $\tilde{\varepsilon}_{\boldsymbol{p}}$ by

$$\tilde{\varepsilon}_{\boldsymbol{p}} = \varepsilon_{\boldsymbol{p}} - \sum_q \frac{\tilde{W}(q)}{i\omega_q - \varepsilon_{\boldsymbol{p}+\boldsymbol{q}} + \varepsilon_{\boldsymbol{p}}}, \tag{15}$$

we can rewrite our scheme into an integral equation to determine $G(p)$ through

$$(i\omega_p - \tilde{\varepsilon}_{\boldsymbol{p}})G(p) = 1 + \sum_q \frac{\tilde{W}(q)G(p+q)}{i\omega_q - \varepsilon_{\boldsymbol{p}+\boldsymbol{q}} + \varepsilon_{\boldsymbol{p}}}. \tag{16}$$

On the assumption of $\bar{I}(q) = 0$, 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 [43,44] or higher dimensional models with strong forward scatterings [45]. This coincidence clearly demonstrates the intrinsically non-perturbative nature of our framework.

In principle, $\bar{I}(q)$ is at our disposal, but Equation (10) suggests us to choose $\bar{I}(q) = -G_+(q)V(\mathbf{q})$ 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 $\Pi_{WI}(q)$. Fortunately, we already know a good form for $G_+(q)$ with taking account of this difference, which is $G_s(q)$ in [22], satisfying the exact limit due to Niklasson [46] as $|\boldsymbol{q}| \to \infty$. The self-consistent results for the homogeneous electron gas up to $r_s = 8$ with this choice of $\bar{I}(q)$ are given in [23].

In the crystalline case, each quantity involved in the $\mathrm{G}\tilde{\mathrm{W}}\Gamma_{\mathrm{WI}}$ scheme should be represented in the matrix form with respect to the reciprocal lattice vectors $\{\boldsymbol{K}\}$. For example, $G(p)$ is a matrix composed of the elements $\{G_{\boldsymbol{K},\boldsymbol{K}'}(\boldsymbol{p}, i\omega_p)\}$ with $\boldsymbol{p}$ 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, $\Pi_{0\,\boldsymbol{K},\boldsymbol{K}'}(q)$ is given as

$$\Pi_{0\,\boldsymbol{K},\boldsymbol{K}'}(q) = \sum_{nn'\boldsymbol{p}\sigma} \frac{f(\varepsilon_{n'\boldsymbol{p}+\boldsymbol{q}}) - f(\varepsilon_{n\boldsymbol{p}})}{i\omega_q - \varepsilon_{n'\boldsymbol{p}+\boldsymbol{q}} + \varepsilon_{n\boldsymbol{p}}} \times \left\langle n\boldsymbol{p}|e^{-i(\boldsymbol{q}+\boldsymbol{K})\cdot\boldsymbol{r}}|n'\boldsymbol{p}+\boldsymbol{q}\right\rangle \left\langle n'\boldsymbol{p}+q|e^{i(\boldsymbol{q}+\boldsymbol{K}')\cdot\boldsymbol{r}'}|n\boldsymbol{p}\right\rangle, \tag{17}$$

where $|n\boldsymbol{p}\rangle$ is the Bloch function for the $n$th band [47,48].

With this understanding, we can apply the $\mathrm{G}\tilde{\mathrm{W}}\Gamma_{\mathrm{WI}}$ scheme to semiconductors and insulators possessing a gap in the electronic excitation energies. Then, without detailed computations, the self-consistently determined quasi-particle energy $E_p$ in this scheme is found to be well approximated by that in the $\mathrm{G_0W_0}$ approximation, as we shall explain in the following.

Let us assume that $\Pi_{\mathrm{WI}}(q) = \Pi_0(q)$ and $\bar{I}(q) = 0$ for the time being. Then, we may rewrite Equation (12) as

$$\Sigma(p) = -\sum_q \frac{W_0(q)}{G_0(p+q)^{-1} - G_0(p)^{-1}} + \gamma(p)G(p)^{-1}, \tag{18}$$

with $W_0(q) \equiv V(\boldsymbol{q})/[1 + V(\boldsymbol{q})\Pi_0(q)]$ and $\gamma(p)$ a dimensionless function, defined by

$$\gamma(p) \equiv \gamma(\boldsymbol{p}, i\omega_p) = \sum_q \frac{G(p+q)W_0(q)}{i\omega_q - \varepsilon_{\boldsymbol{p}+\boldsymbol{q}} + \varepsilon_{\boldsymbol{p}}}. \tag{19}$$

The quasi-particle dispersion $E_{\boldsymbol{p}}$ is determined by the pole of the retarded one-electron Green's function $G^R(\boldsymbol{p}, \omega)$, or $G^R(\boldsymbol{p}, E_{\boldsymbol{p}})^{-1} = 0$, amounting to $E_{\boldsymbol{p}} = \varepsilon_{\boldsymbol{p}} + \Sigma^R(\boldsymbol{p}, E_{\boldsymbol{p}})$, where we obtain the 'on-shell' retarded self-energy as

$$\Sigma^R(\boldsymbol{p}, E_{\boldsymbol{p}}) = -\sum_q \frac{W_0(q)}{i\omega_q - \varepsilon_{\boldsymbol{p}+\boldsymbol{q}} + \varepsilon_{\boldsymbol{p}}}, \tag{20}$$

by analytic continuation of $\Sigma(p)$ in Equation (18). In deriving Equation (20), we have paid due attention to the convergence of $\gamma^R(\boldsymbol{p}, E_{\boldsymbol{p}})$ in gapful systems. In fact, provided that $\bar{I}(q) = 0$, $\tilde{\varepsilon}_{\boldsymbol{p}}$ and the integral in the right-hand side in Equation (16) are, respectively, reduced to $E_{\boldsymbol{p}}$ and $\gamma(p)$, leading to the behaviour of $G^R(\boldsymbol{p}, \omega)$ for $\omega$ near $E_{\boldsymbol{p}}$ as

$$G^R(\boldsymbol{p}, \omega) \approx \frac{1 + \gamma^R(\boldsymbol{p}, E_{\boldsymbol{p}})}{\omega + i0^+ - E_{\boldsymbol{p}}}. \tag{21}$$

For comparison, let us consider the self-energy in the $\mathrm{G_0W_0}$ approximation, which is given by $\Sigma_0(p) = -\Sigma_q G_0(p+q)W_0(q)$. By analytic continuation $i\omega_p \to \epsilon_{\boldsymbol{p}} + i0^+$, we obtain

$$\Sigma_0^R(\boldsymbol{p}, \varepsilon_{\boldsymbol{p}}) = -\sum_q \frac{W_0(q)}{i\omega_q - \varepsilon_{\boldsymbol{p}+\boldsymbol{q}} + \varepsilon_{\boldsymbol{p}}} - \frac{1}{2}\sum_{\boldsymbol{q}} W_0(\boldsymbol{q}, \varepsilon_{\boldsymbol{p}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{p}}) \times \left[\coth\frac{\varepsilon_{\boldsymbol{p}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{p}}}{2T} - \tanh\frac{\varepsilon_{\boldsymbol{p}+\boldsymbol{q}}}{2T}\right]. \tag{22}$$

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Because the transition $\boldsymbol{p}+\boldsymbol{q} \to \boldsymbol{p}$ involved in Equation (22) is relevant only for the interband transition, $|\varepsilon_{\boldsymbol{p}+\boldsymbol{q}}-\varepsilon_{\boldsymbol{p}}|$ is always larger than $E_g$ the energy gap. At low $T$, the chemical potential $\mu$ lies at the centre of the band gap, indicating that $|\varepsilon_{\boldsymbol{p}+\boldsymbol{q}}| \geq E_g/2$. These two facts allow us to safely neglect the contribution from the second sum in Equation (22), as long as $T \ll E_g$. Thus, we may write $E^0_{\boldsymbol{p}}$ the quasi-article dispersion in the $G_0W_0$ approximation as

$$E^0_{\boldsymbol{p}} = \varepsilon_{\boldsymbol{p}} + \Sigma^R_0(\boldsymbol{p}, \varepsilon_{\boldsymbol{p}}) = \varepsilon_{\boldsymbol{p}} - \sum_q \frac{W_0(q)}{i\omega_q - \varepsilon_{\boldsymbol{p}+\boldsymbol{q}} + \varepsilon_{\boldsymbol{p}}}, \quad (23)$$

leading us to conclude that $E^0_{\boldsymbol{p}} = E_{\boldsymbol{p}}$. Note, however, that the spectral weight $z_{\boldsymbol{p}}$ $[= (1-\partial\Sigma^R_0(\boldsymbol{p}, \omega)/\partial\omega)^{-1}|_{\omega=\varepsilon_{\boldsymbol{p}}}]$ is different from $1+\gamma^R(\boldsymbol{p}, E_{\boldsymbol{p}})$.

In the literature, $E^0_{\boldsymbol{p}}$ is sometimes evaluated as $E^0_{\boldsymbol{p}} = \varepsilon_{\boldsymbol{p}} + z_{\boldsymbol{p}}\Sigma^R_0(\boldsymbol{p}, \varepsilon_{\boldsymbol{p}})$ and there is a controversy as to whether this $z_{\boldsymbol{p}}$ should be included or not. As previously discussed in detail [29], we consider it better not to include $z_{\boldsymbol{p}}$ 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 $E^0_{\boldsymbol{p}} = E_{\boldsymbol{p}}$ without this factor $z_{\boldsymbol{p}}$ indicates that this feature of mutual cancellation reaches far up to infinite order in semiconductors and insulators.

Finally, we comment on the two assumptions as well as other related issues. (i) The difference between $\Pi_{WI}$ and $\Pi_0$ arises only from that between $n(\boldsymbol{p})$ and $f(\varepsilon_{\boldsymbol{p}})$. In usual semiconductors and insulators, the valence-electron density is high; for example, $r_s = 2$ for Si. Now $n(\boldsymbol{p})$ in a metal at such $r_s$ does not deviate much from $f(\varepsilon_{\boldsymbol{p}})$ except for the states near the Fermi level, as shown in Figure 4 in [23], but those states are absent from the outset in these gapful systems. Thus, $n(\boldsymbol{p})$ is close to $f(\varepsilon_{\boldsymbol{p}})$, leading to $\Pi_{WI} \approx \Pi_0$. (ii) Justification of $\bar{I} = 0$ has already been done by numerical studies in [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 $|\boldsymbol{q}|$ for principal processes is of the order of $|\boldsymbol{K}|$, making $V(\boldsymbol{q})$ very small and $G_+(q)$ reach its asymptotic constant. Thus, the effect of $\bar{I}$ is weak in semiconductors and insulators. (iii) The inherent problem in the $G_0W_0$ approximation is the dependence of the results on the arbitrary starting basis. From our perspective, the dependence originates from the degree of satisfying the above two assumptions. Thus, if the gap energies (or the vertical ionisation potentials (IPs) for atoms and molecules) are large enough, the dependence becomes small and the results in the $G_0W_0$ approximation from any starting point are close to the experimental values, as seen for IPs of He and Ne in Table V in [15] and of CO and $N_2$ in Table I in [13]. (iv) We have shown that the $G_0W_0$ approximation is good for obtaining the quasi-particle dispersion for gapful systems, but there is no guarantee for other physical quantities such as the line shape of $A(\boldsymbol{p}, \omega)$. On the other hand, the framework stipulated by the set of equations (Equations (2)–(8)) is, in principle, exact and can provide accurate results for the physical quantities directly derived from $G(p)$. Thus, the physical requirements such as the non-negativity of $A(\boldsymbol{p}, \omega)$ are automatically satisfied, as long as we choose an appropriate approximation to $\tilde{I}(p+q, p; p'+q, p')$ which is a single quantity in the framework to control the accuracy of the results. We can determine a proper functional form for $\tilde{I}(p+q, p; p'+q, p')$ by the use of the information on the local-field factor or by perturbation expansion from either weak or strong coupling limit, supplemented by the information obtained by quantum Monte Carlo simulations, if available.

## 3. Superconducting state

In the conventional phonon mechanism of superconductivity with spin-singlet $s$-wave Cooper pairing, we can formulate the problem in much the same way as in the normal state, if we employ the Nambu representation [49]. We obtain the rigorous expressions for $\Pi(q)$ and $\Sigma(p)$ as

$$\Pi(q) = -\sum_p \mathrm{Tr}\left[\tau_3 G(p+q)\Gamma(p+q, p)G(p)\right], \quad (24)$$

$$\Sigma(p) = -\sum_q \tau_3 G(p+q)\Gamma(p+q, p)W(q), \quad (25)$$

respectively. They are very similar to Equations (2) and (3), but $\Sigma(p)$, together with the scalar vertex function $\Gamma(p+q, p)$, is now a $2 \times 2$ matrix. Here, $\tau_i$s for $i$=1, 2, and 3 are the usual $2 \times 2$ Pauli matrices and $W(q)$ is the effective electron–electron interaction. For the electron–phonon coupled system, $W(q)$ is exactly obtained as

$$W(q) = \frac{V(\boldsymbol{q}) + V_{\mathrm{ph}}(q)}{1 + [V(\boldsymbol{q}) + V_{\mathrm{ph}}(q)]\Pi(q)}, \quad (26)$$

where $V_{\mathrm{ph}}(q)$ is the bare phonon-mediated electron-electron interaction, given by

$$V_{\mathrm{ph}}(q) = \sum_\nu |g_{\boldsymbol{q}\nu}|^2 \frac{2\Omega_{\boldsymbol{q}\nu}}{(i\omega_q)^2 - \Omega_{\boldsymbol{q}\nu}{}^2}, \quad (27)$$

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with bare electron–phonon coupling $g_{\boldsymbol{q}\nu}$ and bare phonon energy $\Omega_{\boldsymbol{q}\nu}$ for the $\nu$th phonon. In this Nambu representation, the WI is written in the form of

$$\begin{aligned}&\left(i\omega_{p'} - i\omega_p\right)\Gamma(p', p) - (\boldsymbol{p}' - \boldsymbol{p})\cdot\boldsymbol{\Gamma}(p', p)\\ &\quad = G(p')^{-1}\tau_3 - \tau_3 G(p)^{-1},\end{aligned} \tag{28}$$

where $\boldsymbol{\Gamma}(p', p)$ is the vector vertex function. Without loss of generality, the $2 \times 2$ matrix $\Sigma(p)$ can be decomposed into

$$\Sigma(p) = [1 - Z(p)]i\omega_p\tau_0 + \phi(p)\tau_1 + \chi(p)\tau_3, \tag{29}$$

with $\tau_0$ the unit matrix. Then, we may rewrite Equation (28) into the form as

$$\begin{aligned}&(i\omega_{p'} - i\omega_p)\Gamma(p', p) - (\boldsymbol{p}' - \boldsymbol{p})\cdot\boldsymbol{\Gamma}(p', p)\\ &\quad = [i\omega_{p'}Z(p') - i\omega_p Z(p)]\tau_3 - [\tilde{\varepsilon}(p') - \tilde{\varepsilon}(p)]\tau_0\\ &\quad + \left[\phi(p') + \phi(p)\right]i\tau_2,\end{aligned} \tag{30}$$

with $\tilde{\varepsilon}(p)$ defined by $\tilde{\varepsilon}(p) \equiv \varepsilon_{\boldsymbol{p}} + \chi(p)$.

Now let us assume that the average phonon energy $\langle\Omega\rangle$ is much smaller than the Fermi energy $\varepsilon_F$ of conduction electrons, as is usually the case for superconductors in the phonon mechanism. In this situation, it is physically relevant to separate the purely Coulombic part from $W(q)$ in Equation (26) in such a way as

$$\begin{aligned}W(q) = &\frac{V(\boldsymbol{q})}{1 + V(\boldsymbol{q})\Pi(q)} + \frac{1}{[1 + V(\boldsymbol{q})\Pi(q)]^2}\\ &\times \frac{V_{\rm ph}(q)}{1 + V_{\rm ph}(\boldsymbol{q})\Pi(q)/[1 + V(\boldsymbol{q})\Pi(q)]}.\end{aligned} \tag{31}$$

In Equation (31), the second term represents the fully screened phonon-mediated interaction, which is supposed to play a central role in bringing about superconductivity. Because this interaction works only in the energy range of about $\langle\Omega\rangle$, the purely Coulombic term, which extends over the range of $\varepsilon_F$, is usually renormalised and reduced into the Coulomb pseudopotential $\mu^*$ which is supposed to work only in the range of about $\langle\Omega\rangle$ in the gap equation to determine $T_c$ [37]. The actual value for $\mu^*$ will be determined phenomenologically in order to reproduce the experimental value of $T_c$. Upon these assumptions, $W(q)$ is not zero only in the vicinity of the Fermi level. This situation can well be treated by the introduction of the cut-off energy $\omega_c$ ($\ll \varepsilon_F$) in considering the sum over momentum $\boldsymbol{p}$ in such a way as

$$\begin{aligned}\sum_{\boldsymbol{p}} &= \int N(\varepsilon)d\varepsilon, \ \text{with}\ N(\varepsilon)\\ &\equiv \sum_{\boldsymbol{p}} \delta(\varepsilon - \varepsilon_{\boldsymbol{p}}) = \begin{cases} N(0) & \text{for } |\varepsilon| < \omega_c,\\ 0 & \text{otherwise,}\end{cases}\end{aligned} \tag{32}$$

where $N(\varepsilon)$ is the electronic density of states per one spin.

Traditionally, a further simplification is made by assuming that $W(q)$ is independent of $\boldsymbol{q}$. Then, $W(q) = W(i\omega_q)$ is written in terms of $\alpha^2F(\Omega)$, the so-called Eliashberg function as

$$\begin{aligned}W(i\omega_q) &= \frac{\mu^* - \lambda(\omega_q)}{N(0)}\\ \text{with}\ \lambda(\omega_q) &\equiv \int_0^\infty d\Omega\, \alpha^2F(\Omega)\, \frac{2\Omega}{{\omega_q}^2 + \Omega^2}.\end{aligned} \tag{33}$$

Note that $\lambda = \lambda(0)$ is the usual non-dimensional electron–phonon coupling constant, and $\langle\Omega\rangle$ is given by

$$\langle\Omega\rangle = \frac{2}{\lambda}\int_0^\infty d\Omega\, \alpha^2F(\Omega). \tag{34}$$

The definition of the Eliashberg function and its calculated results on various superconductors are available in the literature [50], but in recent years we can obtain the results rather easily by using the packages for first-principles calculations such as Quantum Espresso [51]. In Figure 2, we show an example of the calculated $\alpha^2F(\Omega)$, which is obtained for fcc Al with the mesh of $48 \times 48 \times 48$ for $\boldsymbol{p}$ and $16 \times 16 \times 16$ for $\boldsymbol{q}$ in the first Brilouin zone.

Incidentally, under the condition of the momentum-independent interaction in Equation (33) and the

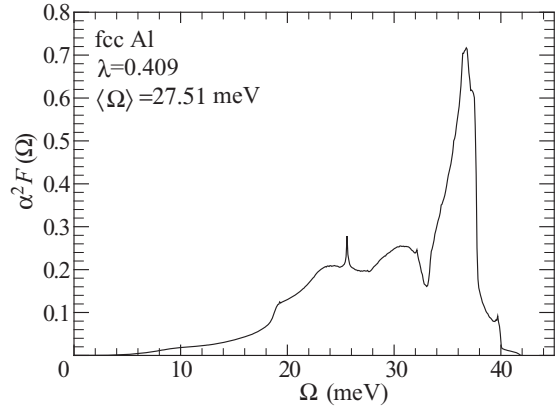


**Figure 2.** The Eliashberg function for fcc Al.

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electron–hole symmetric situation as suggested in Equation (32), the level-shift function $\chi(p)$ in Equation (29) is easily found to be zero. The renormalisation function $Z(p)$ and the gap function $\phi(p)$ are not zero but independent of the momentum variable $\boldsymbol{p}$. Then, we can assume that the scalar vertex function is also independent of momentum variables and it must obey the relation, given by

$$(i\omega_{p'} - i\omega_p)\Gamma(i\omega_{p'}, i\omega_p) = [i\omega_{p'}Z(i\omega_{p'}) - i\omega_p Z(i\omega_p)]\tau_3 + \left[\phi(i\omega_{p'}) + \phi(i\omega_p)\right] i\tau_2. \quad (35)$$

This relation is derived by setting $\boldsymbol{p}' = \boldsymbol{p}$ in Equation (30) and indicates that $\Gamma(i\omega_{p'}, i\omega_p)$ contains the $\tau_2$-component. As originally discussed by Nambu [49], this component is related to the phase-collective Nambu–Goldstone mode. In superconductors, the energy of this mode is the plasmon energy $\omega_{\rm pl}$, which is the energy scale far beyond $\langle\Omega\rangle$. Thus, we will omit this contribution to the vertex function in the present treatment in which all physical quantities beyond the energy scale $\langle\Omega\rangle$ will be neglected with the hope that due effects will be renormalised and included into the definition of $\mu^*$. There are also discussions on the $\tau_1$-component in the vertex function, which is related to the amplitude-collective Nambu–Goldstone mode [52,53], but it is known that this contribution does not change $T_c$ [54], assuring us of neglecting it altogether in the calculation of $T_c$. Thus we obtain $\Gamma(i\omega_{p'}, i\omega_p)$ as

$$\Gamma(i\omega_{p'}, i\omega_p) = \frac{i\omega_{p'}Z(i\omega_{p'}) - i\omega_p Z(i\omega_p)}{i\omega_{p'} - i\omega_p}\,\tau_3, \quad (36)$$

for $\omega_{p'} \neq \omega_p$. At $\omega_{p'} = \omega_p$, we cannot use the WI to determine it, but on general considerations, it is given by $[1 - \delta\Sigma(p)/\delta\mu]\tau_3$ with the normal-state self-energy $\Sigma(p)$ and $\mu$ the Fermi level, which is different from $\lim_{\omega_{p'}\to\omega_p}\Gamma(i\omega_{p'}, i\omega_p)$ in Equation (36). In this paper, however, we shall use this limit, i.e. $\Gamma(i\omega_p, i\omega_p) = [Z(i\omega_p) + \omega_p\delta Z(i\omega_p)/\delta\omega_p]\tau_3$, partly because no appropriate information on $\delta\Sigma(p)/\delta\mu$ is available and partly because we know that this difference, which appears only in a single term in the infinite sum of $T\sum_{\omega_{p'}}$, becomes very important only when the small polaronic effect is large [55].

By summarising all the above assumptions and considerations, we can derive a couple of equations, one for $Z(i\omega_p)$ and the other for $\phi(i\omega_p)$, to determine $T_c$ by retaining only up to the linear order in $\phi(p)$ in Equation (25) in the following way:

$$Z(i\omega_p) = 1 + \frac{2T}{\omega_p}\sum_{\omega_{p'}}\lambda(\omega_{p'} - \omega_p)\Gamma(i\omega_{p'}, i\omega_p) \times \tan^{-1}\left[\frac{\omega_c}{\omega_{p'}Z(i\omega_{p'})}\right], \quad (37)$$

$$\Delta(i\omega_p) = \frac{2T}{Z(\omega_p)}\sum_{\omega_{p'}}\frac{\Delta(i\omega_{p'})}{\omega_{p'}}[\lambda(\omega_{p'} - \omega_p) - \mu^*] \times \Gamma(i\omega_{p'}, i\omega_p)\tan^{-1}\left[\frac{\omega_c}{\omega_{p'}Z(i\omega_{p'})}\right], \quad (38)$$

where $\Delta(i\omega_p)$ is defined by $\phi(i\omega_p)/Z(i\omega_p)$. We can define $T_c$ by the highest temperature at which non-zero $\Delta(i\omega_p)$ can be found. We shall call $T_c$ obtained from these equations a result in the GISC scheme. In the Eliashberg theory, $T_c$ is determined by the solution of Equations (37) and (38) with taking $\Gamma(i\omega_{p'}, i\omega_p) = 1$. Usually, the Eliashberg function $\alpha^2F(\Omega)$ is not renormalised in the process of self-consistently determining $Z(i\omega_p)$. In this sense, the Eliashberg theory might be better regarded as the '$GW_0$' approximation, rather than the GW one. If we do not solve Equation (37) for $Z(i\omega_p)$ but simply take $Z(i\omega_p) = 1$ in the solution of Equation (38), the obtained $T_c$ may be considered as a result in the $G_0W_0$ approximation.

By using the $\alpha^2F(\Omega)$ function in Figure 2, we have calculated $T_c$ for fcc Al in three different schemes and shown the results as a function of $\mu^*$ in the Eliashberg theory (solid curve), the GISC (dashed curve), and the $G_0W_0$ (dotted curve) in Figure 3. Note that this is a typical example for the weakly correlated and weakly coupled superconductors. The cut-off energy $\omega_c$ is increased up to $5\langle\Omega\rangle$ in order to obtain the convergent results for $T_c$. As can be seen in Figure 3, $T_c$ in the most sophisticated GISC scheme is very different from that in the Eliashberg theory but very close to that in the simplest scheme of the

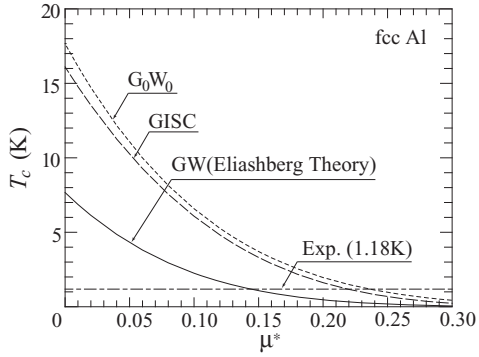


**Figure 3.** Superconducting transition temperature $T_c$ for fcc Al as a function of the Coulomb pseudopotential $\mu^*$ in three different calculation schemes in comparison with the experimental $T_c$ of 1.18 K.

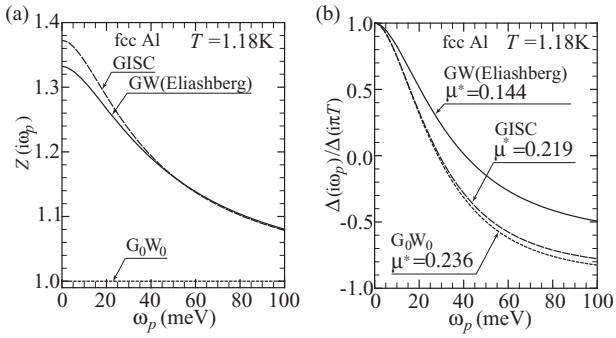


**Figure 4.** (a) Renormalisation factor $Z(i\omega_p)$ and (b) the gap function $\Delta(i\omega_p)$ normalised by $\Delta(i\pi T)$ calculated for fcc Al at $T =$ 1.18 K in the three different schemes.

$G_0W_0$, indicating that the vertex corrections included in the GISC is mostly cancelled by the self-energy renormalisation corrections.

Because the experimental value of $T_c$ for fcc Al is 1.18 K, we can determine the value of $\mu^*$ for each scheme; they are 0.144, 0.219 and 0.236 for the Eliashberg, the GISC and the $G_0W_0$, respectively. Then, we can compare the results for $Z(i\omega_p)$ and $\Delta(i\omega_p)/\Delta(i\pi T)$ at $T =$ 1.18 K, as shown in Figure 4. Although the Eliashberg and the GISC provide more or less the same $Z(i\omega_p)$, the results for $\Delta(i\omega_p)/\Delta(i\pi T)$ are very different. We see that as far as the superconducting properties are concerned, the $G_0W_0$ gives about the same quality of results as the GISC.

Four comments are in order. (i) According to the Migdal's theorem [56], one might expect that the Eliashberg theory gives approximately the same $T_c$ as the GISC for such weakly coupled conventional superconductors because of the irrelevance of the vertex corrections. A closer inspection of the Migdal's proof reveals, however, that the theorem states only the irrelevance of the first-order vertex corrections, but not for the first-order self-energy corrections. If the irrelevance of the former corrections is true, the same must be true for the latter, given that the WI always holds. In this regard, the Migdal's theorem actually proves the relevance of the $G_0W_0$ approximation, which is indeed confirmed by the results in Figure 3. (ii) The preference of the $G_0W_0$ approximation to the Eliashberg theory applies only to the calculation of $T_c$; the normal-state property in a metal as represented by $Z(i\omega_p)$ is better described by the latter, as can be seen in Figure 4(a). (iii) Since $T_c$ in all the three schemes varies very much with the change of $\mu^*$, those schemes are not good enough for the first-principles calculation of $T_c$, as long as $\mu^*$ is given phenomenologically. Thus, we need to develop a scheme to determine $\mu^*$ from first principles. The present author pursued such a scheme in the framework of the $G_0W_0$ approximation [57], according to which the gap function is not considered as a function of the frequency variable but the momentum one and the gap equation to give $T_c$ is derived for the momentum-dependent gap function $\Delta(\boldsymbol{p})$ as

$$\Delta(\boldsymbol{p}) = -\sum_{\boldsymbol{p}'} \frac{\Delta(\boldsymbol{p}')}{2\varepsilon_{\boldsymbol{p}'}} \tanh\left(\frac{\varepsilon_{\boldsymbol{p}'}}{2T_c}\right) \mathcal{K}_{\boldsymbol{p},\boldsymbol{p}'}, \tag{39}$$

where the pairing interaction $\mathcal{K}_{\boldsymbol{p},\boldsymbol{p}'}$ is defined by

$$\mathcal{K}_{\boldsymbol{p},\boldsymbol{p}'} = \int_0^\infty \frac{2}{\pi} d\Omega \frac{|\varepsilon_{\boldsymbol{p}}| + |\varepsilon_{\boldsymbol{p}'}|}{\Omega^2 + (|\varepsilon_{\boldsymbol{p}}| + |\varepsilon_{\boldsymbol{p}'}|)^2} W(\boldsymbol{p}-\boldsymbol{p}', i\Omega), \tag{40}$$

with $W(q)$ given by Equation (26) in which $\Pi(q)$ is replaced by $\Pi_0(q)$. This scheme was successfully applied to real materials such as the $n$-type $SrTiO_3$ [58] and the graphite intercalation compounds [59,60]. (iv) First-principles determination of $\mu^*$ is also made possible by SCDFT [38–41], according to which the fundamental gap equation is just the same as that in Equation (39), but the pairing interaction is different from the one in Equation (40). Because the form in Equation (40) includes the contribution from the plasmons [57] in a very natural way [61,62], it is strongly recommended to employ Equation (40) for future implementation of SCDFT [63].

## 4. Conclusion

In summary, we have discussed the relevance of the $G_0W_0$ approximation in obtaining some of physical quantities in both normal and superconducting states. Due to the existence of the WI, this approximation remains to be useful in a much wider interaction range than one might naively imagine, probably up to the medium coupling range in which most of the real materials are involved.

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