

Inclusion of Vertex Corrections in the Self-Consistent Calculation of Quasiparticles in Metals

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Based on the Bethe-Salpeter equation and the Ward identity derived from it, we provide a scheme for constructing the vertex function in the self-consistent iteration loop to determine the electron self-energy. The scheme is implemented in the homogeneous electron gas at the sodium density.

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Angle-resolved photoemission spectroscopy (ARPES) experiments provide invaluable information on the electronic structure of a material. Conventionally ARPES is analyzed on the assumption that the final state is well described by the free-electron model [1]. In their recent Letter [2], Yasuhara *et al.* threw doubt on the validity of this assumption; they claimed that the interacting electron-gas model should be used instead. Since it touched upon one of the fundamental issues in condensed-matter physics, their claim invited much debate. For example, Ku *et al.* [3] raised a problem of the lack of self-consistency in determining the self-energy Σ in Ref. [2]. In this Letter we report substantial progress on this problem.

A canonical self-consistent calculation scheme for Σ in solids has been formulated by Hedin [4] who advocates the so-called *GW* approximation (GWA) [5]. In the early stage of actual calculations, Σ was evaluated without self-consistency in the electron Green's function G , namely, with $G = G^{(0)}$, and the dynamically screened interaction W was approximated to $W^{(0)}$ the effective interaction in the random-phase approximation (RPA). This simplest $G^{(0)}W^{(0)}$ treatment yielded the results in apparently good agreement with experiments such as the bandwidth narrowing in alkali metals [6]. In recent years, a faithful implementation of GWA has become feasible at least in the electron gas [7–9], as well as in simple metals and semiconductors [10]. This elaboration, however, has made the results deviate from experiments, indicating the

complicated situation in which the self-consistency should be sought in conjunction with the vertex corrections.

Since a lack of the vertex function Γ is well recognized as a major drawback of GWA, there have been many attempts to include Γ in the calculation of Σ , usually abbreviated to *GW Γ* . There are three avenues to Γ : (a) term-by-term calculation of low-order corrections in W [11], (b) estimation of Γ using the local-field factor [7,12], and (c) systematic construction of Γ by an iterative procedure [13]. In this Letter, we propose a hybrid scheme for Γ combining merits of these approaches without increasing computational cost much from that for GWA.

Using this scheme, we have performed the self-consistent calculation of Σ in *GW Γ* for the electron gas, from which we can derive the quasiparticle energy dispersion. Assuming the interacting electron-gas model for the final state in analyzing ARPES as in Ref. [2], we obtain a very good agreement between theory and experiment.

The Dyson equation relates $G(p)$ the one-electron thermal Green's function with $G^{(0)}(p)$ the bare one through

$$G(p)^{-1} \equiv G_{\sigma}(\mathbf{p}, i\omega_n)^{-1} = G^{(0)}(p)^{-1} - \Sigma(p), \quad (1)$$

where p is used as a combined notation of momentum $\mathbf{p} \equiv (p_1, p_2, p_3)$, spin σ , and fermion Matsubara frequency $i\omega_n \equiv i\pi T(2n + 1)$ at temperature T with an integer n [14]. The Bethe-Salpeter equation determines the three-point vertex function $\Gamma_{\alpha,\nu}(p, p + q)$ in both charge ($\alpha = +$) and spin ($\alpha = -$) channels as

$$\Gamma_{\alpha,\nu}(p, p + q) = \gamma_{\nu}(p, p + q) + T \sum_{\omega_n'} \sum_{\mathbf{p}'\sigma'} \tilde{I}_{\alpha}(p, p + q; p', p' + q) G(p') G(p' + q) \Gamma_{\alpha,\nu}(p', p' + q), \quad (2)$$

where $\nu = 0$ indicates the scalar part while $\nu = 1, 2$, and 3 the vector part, q denotes the combination of momentum \mathbf{q} and boson Matsubara frequency $i\omega_l \equiv 2i\pi Tl$ with an integer l , $\gamma_{\nu}(p, p + q)$ is the bare three-point vertex, and $\tilde{I}_{\alpha}(p, p + q; p', p' + q)$ is the electron-hole four-point irreducible interaction in the channel α . From Eq. (2), we can derive the Ward identity (WI), representing the local electron-number conservation law, as

$$i\omega_l \Gamma_{\alpha,0}(p, p + q) - |\mathbf{q}| \Gamma_{\alpha,lv}(p, p + q) = G(p + q)^{-1} - G(p)^{-1}, \quad (3)$$

with $\Gamma_{\alpha,lv}(p, p + q)$ the longitudinal vector vertex part, defined by $\Gamma_{\alpha,lv}(p, p + q) \equiv \sum_{\nu=1}^3 q_{\nu} \Gamma_{\alpha,\nu}(p, p + q) / |\mathbf{q}|$.

Introducing the function $R_{\alpha}(p, p + q)$, defined by

$$R_{\alpha}(p, p + q) \equiv \frac{\Gamma_{\alpha,0}(p, p + q) \sum_{\nu=1}^3 q_{\nu} \gamma_{\nu}(p, p + q)}{|\mathbf{q}| \Gamma_{\alpha,lv}(p, p + q)}, \quad (4)$$

we can rewrite Eq. (3) into

$$\Gamma_{\alpha,0}(p, p + q) = \frac{G(p + q)^{-1} - G(p)^{-1}}{i\omega_l - (\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}}) / R_{\alpha}(p, p + q)}, \quad (5)$$

where use is made of the fact that $\sum_{\nu=1}^3 q_{\nu} \gamma_{\nu}(p, p + q) = \epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}}$ with $\epsilon_{\mathbf{p}}$ the bare one-electron dispersion.

Similarly, $\Gamma_{\alpha,lv}(p, p + q)$ is given in terms of $R_{\alpha}(p, p + q)$ as

$$\Gamma_{\alpha,lv}(p, p + q) = \frac{G(p + q)^{-1} - G(p)^{-1}}{|\mathbf{q}|[-1 + R_{\alpha}(p, p + q)i\omega_l/(\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}})]}. \quad (6)$$

According to the Fermi-liquid theory [15], appropriate sum rules or conservation laws determine the exact values for $R_{\alpha}(p, p + q)$ at the Fermi surface ($|\mathbf{p}| = p_F$) in both the ω limit ($\mathbf{q} = \mathbf{0}$ and then $\omega_l \rightarrow 0$) and the \mathbf{q} limit ($\omega_l = 0$ and then $\mathbf{q} \rightarrow \mathbf{0}$). In fact, $R_{\alpha}(p, p + q)$ tends to unity in the ω limit, while in the \mathbf{q} limit we obtain

$$\begin{aligned} R_+(p, p + q) &\rightarrow \kappa/\kappa^{(0)}, \\ \text{and } R_-(p, p + q) &\rightarrow \chi/\chi^{(0)}, \end{aligned} \quad (7)$$

where κ and χ are, respectively, the compressibility and the spin susceptibility with $\kappa^{(0)}$ and $\chi^{(0)}$ the respective noninteracting values.

So far everything is formal and exact. Now we resort to an approximation. If we replace $\tilde{I}_{\alpha}(p, p + q; p', p' + q)$ in Eq. (2) by some suitably averaged quantity $\langle \tilde{I}_{\alpha} \rangle_{p,p+q}$ over the variables p' , we obtain

$$\begin{aligned} \Gamma_{\alpha,0}(p, p + q) &= \Gamma_{\alpha,0}^{(a)}(p, p + q) \\ &\equiv 1 - \langle \tilde{I}_{\alpha} \rangle_{p,p+q} \Pi_{\alpha}(q), \end{aligned} \quad (8)$$

$$\begin{aligned} \Gamma_{\alpha,lv}(p, p + q) &= \Gamma_{\alpha,lv}^{(a)}(p, p + q) \\ &\equiv [\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}} \\ &\quad - \langle \tilde{I}_{\alpha} \rangle_{p,p+q} \Pi_{\alpha}(q) i\omega_l] / |\mathbf{q}|, \end{aligned} \quad (9)$$

where $\Pi_{\alpha}(q)$ the polarization function in the channel α is defined in a conventional way as

$$\Pi_{\alpha}(q) = -T \sum_{\omega_n} \sum_{\mathbf{p}\sigma} G(p)G(p + q)\Gamma_{\alpha,0}(p + q, p). \quad (10)$$

In deriving Eq. (9), we have used Eq. (3) to relate $\Pi_{\alpha}(q)$ with the ‘‘longitudinal vector’’ polarization function, defined by Eq. (10) with $\Gamma_{\alpha,lv}$ in place of $\Gamma_{\alpha,0}$. Physically, $\langle \tilde{I}_{\alpha} \rangle_{p,p+q}$ can be understood by the concept of $G_{\pm}(\mathbf{q})$, the exchange-correlation local-field factor [16], or equivalently $f_{\pm,xc}(q)$, the exchange-correlation kernel appearing in the time-dependent density functional theory (TDDFT) [17], indicating that a simple choice for $\langle \tilde{I}_{\alpha} \rangle_{p,p+q}$ is $f_{\alpha,xc}(q)$ or $-G_{\alpha}(\mathbf{q})V(\mathbf{q})$ with $V(\mathbf{q}) = 4\pi e^2/q^2$. Then, approximating $\Pi^{(0)}/(1 + f_{\alpha,xc}\Pi^{(0)})$ to Π_{α} with $\Pi^{(0)}$ the polarization function in RPA, we see that Eq. (8) for $\Gamma_{\alpha,0}$ is reduced to $\Gamma_{\alpha,0} = (1 + f_{\alpha,xc}\Pi^{(0)})^{-1}$, an expression very frequently adopted in the literature [7,12,16].

In spite of its popularity, Eq. (8) combined with Eq. (9) is unsatisfactory in the sense that WI is not fulfilled, no matter how $\langle \tilde{I}_{\alpha} \rangle_{p,p+q}$ is chosen. However, we find that WI is made satisfied, if we determine the vertex parts by Eqs. (5) and (6) through $R_{\alpha}(p, p + q)$ which is approximated to the ratio of Eqs. (8) and (9) as

$$R_{\alpha}(p, p + q) = \frac{\Gamma_{\alpha,0}^{(a)}(p, p + q)(\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}})}{|\mathbf{q}|\Gamma_{\alpha,lv}^{(a)}(p, p + q)}. \quad (11)$$

In fact, substitution of Eq. (11) into Eqs. (5) and (6) pro-

vides the vertex parts as [18]

$$\Gamma_{\alpha,0}(p, p + q) = \Gamma_{\alpha,0}^{(a)}(p, p + q)\Gamma^{(b)}(p, p + q), \quad (12)$$

$$\Gamma_{\alpha,lv}(p, p + q) = \Gamma_{\alpha,lv}^{(a)}(p, p + q)\Gamma^{(b)}(p, p + q), \quad (13)$$

with $\Gamma^{(b)}(p, p + q)$ a functional of G , defined by

$$\Gamma^{(b)}(p, p + q) \equiv \frac{G(p + q)^{-1} - G(p)^{-1}}{G^{(0)}(p + q)^{-1} - G^{(0)}(p)^{-1}}. \quad (14)$$

Because of the factor $\Gamma^{(b)}$, we easily see that Eq. (12) in conjunction with Eq. (13) fulfills WI, irrespective of the form of $\langle \tilde{I}_{\alpha} \rangle_{p,p+q}$. The importance of WI in determining quasiparticle energies has already been illustrated in a toy model [19]. The presence of $\Gamma^{(b)}$ is also physically reasonable, because it ‘‘measures the distance’’ of each electron specified by either p or $p + q$ from the Fermi surface. This feature cannot be described by such a factor as $f_{\pm,xc}(q)$ which depends only on ‘‘the relative distance’’ between these electrons.

Let us apply the above scheme to the interacting homogeneous electron gas in which only the charge channel is relevant in calculating $\Sigma(p)$, given by

$$\Sigma(p) = -T \sum_{\omega_l} \sum_{\mathbf{q}} W(q)G(p + q)\Gamma_{+,0}(p, p + q), \quad (15)$$

with the effective interaction $W(q)$, defined by

$$W(q) = V(\mathbf{q})/[1 + V(\mathbf{q})\Pi_+(q)]. \quad (16)$$

As schematically shown in Fig. 1, the self-consistent iteration loop to determine $\Sigma(p)$ is now completed. Once we specify $\langle \tilde{I}_{+} \rangle_{p,p+q}$, we can actually implement this loop, starting from the noninteracting solution and ending the loop when the relative difference in $\Sigma(p)$ between input and output at each p becomes sufficiently small. We consider the difference small if it is less than 10^{-5} .

A conceptually simple method of making a systematic determination of $\langle \tilde{I}_{+} \rangle_{p,p+q}$ is to employ perturbation theory, expanding the vertex corrections in terms of $W^{(0)}$ [11,20]. Computationally a difficulty arises in calculating higher-order terms. A practical way to remedy this difficulty is to rescale the total magnitude of $\langle \tilde{I}_{+} \rangle_{p,p+q}$ in the lowest-order calculation in order to satisfy Eq. (7) with $R_{\alpha}(p, p + q)$ in Eq. (11), using the accurate values of κ as a function of the electronic density parameter r_s obtained by Monte Carlo simulations [21]. Another

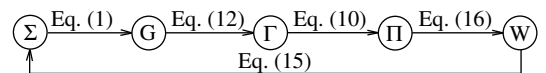


FIG. 1. Iteration loop to determine the self-energy.

method of determining $\langle \tilde{I}_+ \rangle_{p,p+q}$ is to use the local-field factor $f_{+,xc}(q)$, in which Eq. (7) is made satisfied by hand in constructing $f_{+,xc}(q)$. We have made many trials in both methods and found that the best choice for $\langle \tilde{I}_+ \rangle_{p,p+q}$ is $f_{xc}^{\text{hom}}(\mathbf{q}, i\omega_l)$ employed in TDDFT, although the final results for $\Sigma(p)$ and concomitant $\Pi_+(q)$ are not very sensitive to the details of $\langle \tilde{I}_+ \rangle_{p,p+q}$, as long as Eq. (7) is fulfilled. The actual form for $f_{xc}^{\text{hom}}(\mathbf{q}, \omega)$ is given explicitly in Sec. 6.1 in Ref. [22]. One of its characteristic features is that $f_{xc}^{\text{hom}}(\mathbf{q}, 0)$ is made equal to $-V(\mathbf{q})G_+(\mathbf{q})$ with the rather accurate local-field factor $G_+(\mathbf{q})$ obtained by Monte Carlo simulations [23]. As for the ω dependence, an interpolation scheme using the Kramers-Kronig relation and the asymptotic behavior of $\text{Im}f_{xc}^{\text{hom}}(\mathbf{q}, \omega) \rightarrow -23\pi/15\omega^{3/2}$ is adopted [17]. Some ambiguity exists in defining $f_{xc}^{\text{hom}}(\mathbf{q}, \omega)$ at finite \mathbf{q} and intermediate values of ω , but a minor modification to $f_{xc}^{\text{hom}}(\mathbf{q}, \omega)$ as explained in Ref. [18] is enough to reproduce the accurate value of the self-energy at the Fermi surface $\Sigma(p_F, 0)$.

With this choice of $\langle \tilde{I}_+ \rangle_{p,p+q}$, we have calculated $\Sigma(\mathbf{p}, i\omega_n)$ as well as $\Pi_+(\mathbf{q}, i\omega_l)$ self-consistently on the imaginary axis in the ω plane for the electron gas with $r_s \leq 5$ at the temperature $T = 0.01E_F$ with E_F the Fermi energy. The obtained values for all static properties are found to agree very well with the respective known accurate ones. To some extent, this is self-evident, because $\langle \tilde{I}_+ \rangle_{p,p+q}$ is so constructed as to reproduce most of them. A nontrivial check on the overall accuracy of $\Sigma(\mathbf{p}, i\omega_n)$ can be made by examining the momentum distribution function $n(\mathbf{p}) [= \lim_{\eta \rightarrow +0} T \sum_{\omega_n} G(p) e^{i\omega_n \eta}]$. Our result for $n(\mathbf{p})$ is in fairly good agreement with the one in the effective-potential expansion (EPX) method, a result considered to be most accurate among various data [24]. (The comparison is made at $r_s = 1$ in Ref. [18].) In the inset (a1) of Fig. 2, our values for z_F , the renormalization factor at the Fermi level or the magnitude of the jump in $n(\mathbf{p})$ at $|\mathbf{p}| = p_F$, are compared with those in EPX, GWA, and the Fermi hypernetted chain method [25].

Analytic continuation onto the real ω axis is needed to obtain $A(\mathbf{p}, \omega) [= -\text{Im}G(\mathbf{p}, \omega)/\pi]$, the one-electron spectral function. This is done with the use of the Padé approximant [26], paying full attention to ensuring analyticity in the upper- ω plane. In actual calculations of $A(\mathbf{p}, \omega)$, instead of genuinely along the real axis, we consider the values at $\omega + i\gamma$ with $\gamma = 0.1\pi T$ so as to make δ -function peaks visible in numerical calculations. In the following we give our results at the sodium density, $r_s = 4$.

In Fig. 2(a), we plot $A(\mathbf{p}, \omega)$ at the Fermi surface. The result in the noninteracting system (the dot-dashed curves) indicates the effect of the artificial width γ on the spectral shape. We see that the quasiparticle represented by the central peak has a vanishingly small width, because the calculated width of the peak is the same as γ . The weight of this δ -function contribution is just z_F . Compared to the partially self-consistent $GW^{(0)}$ calculation (the dashed curve), our result is much closer to that in RPA (the dotted curve). This supports the well-known argument that the

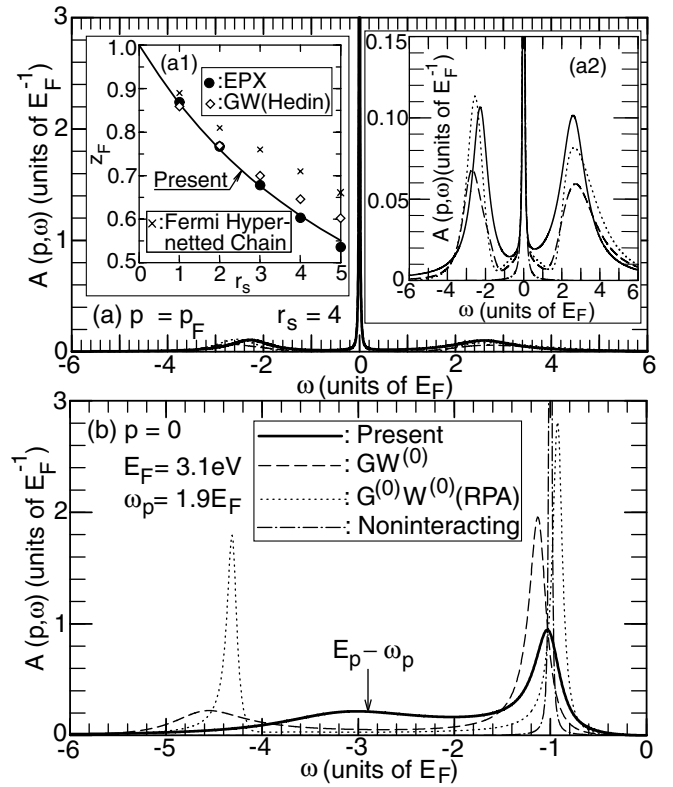


FIG. 2. One-electron spectral function (a) at the Fermi level and (b) at the band bottom. In the inset (a1), our results for z_F as a function of r_s are compared with those in other methods. The inset (a2) gives the magnified $A(\mathbf{p}, \omega)$ at $|\mathbf{p}| = p_F$ to show the detail of plasma sidebands.

self-energy insertion is mostly canceled by the vertex correction, a fact attributable eventually to the Pauli principle [27].

Such a cancellation does not work for $|\mathbf{p}|$ very far away from the Fermi surface, as exemplified in Fig. 2(b) which shows that our result differs very much from that in either RPA or $GW^{(0)}$ at the band bottom. More specifically, our main peak describing the quasiparticle is associated with the width as large as a few tenths of E_F , indicating that the quasiparticle is suffering from a strong damping effect due to the multiple electron-hole pair excitations that are fully included in our treatment. These pair excitations contribute to the long tail in $A(\mathbf{p}, \omega)$ extending to the vague peak corresponding to the plasmaron or the real plasmon coupled to the quasiparticle [4]. Note that the strong damping effect of the plasmaron can be well described even by $GW^{(0)}$, but the correct peak position (namely, E_p , the quasiparticle position minus ω_p , the plasmon energy) can be obtained only through the proper inclusion of vertex corrections [19].

In spite of the strong damping effect, we can identify the quasiparticle peak position E_p at each \mathbf{p} in $A(\mathbf{p}, \omega)$. In the Fig. 3 inset, we plot the quasiparticle self-energy correction, $\Sigma(\mathbf{p}, E_p)$, as a function of $|\mathbf{p}|$. We see that our result for the real part (the solid curve) is very close to that obtained in Ref. [2] (the dot-dashed curve), but it is definitely different from that in RPA (the dotted curve). In

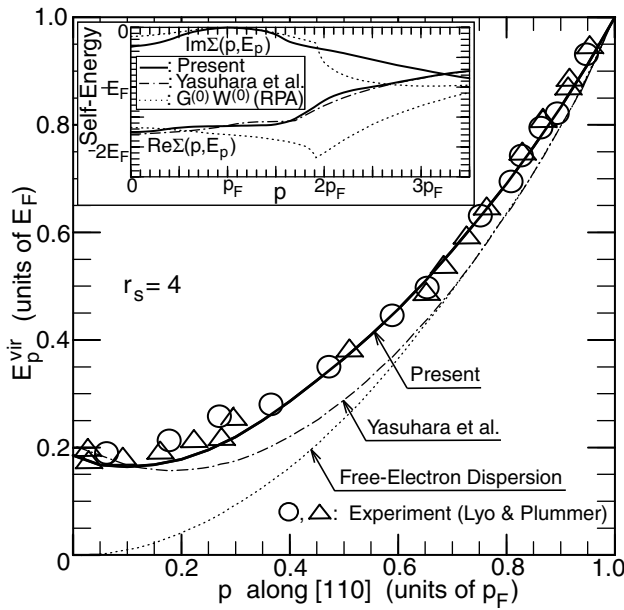


FIG. 3. Comparison between the experimental energy band and the calculated virtual energy band defined in Eq. (17). Inset: Quasiparticle self-energy Σ correction in both real and imaginary parts as a function of $|\mathbf{p}|$ at $r_s = 4$.

particular, our method provides a monotonically increasing $\text{Re}\Sigma(\mathbf{p}, E_p)$ with the increase of $|\mathbf{p}|$, leading to the widening of the occupied bandwidth by about 2%.

An interesting feature is that $\text{Re}\Sigma(\mathbf{p}, E_p)$ is quite flat in the region $0.5p_F < |\mathbf{p}| < 1.5p_F$, implying hindsight that the Slater's $X\alpha$ method or the local-density approximation to DFT works so successfully. Outside of that region, $\text{Re}\Sigma(\mathbf{p}, E_p)$ changes gradually with the concomitant rather rapid increase in $|\text{Im}\Sigma(\mathbf{p}, E_p)|$. For $|\mathbf{p}|$ larger than about $2p_F$, the opening of the plasmon-damping channel makes $\text{Re}\Sigma(\mathbf{p}, E_p)$ change in proportion to $|\mathbf{p}|^{-1}$ [2] and $|\text{Im}\Sigma(\mathbf{p}, E_p)|$ increase further, though no sudden change is seen in our result in contrast to that in RPA.

Since $\text{Re}\Sigma(\mathbf{p}, E_p)$ cannot be neglected even for $|\mathbf{p}|$ as large as $4.5p_F$ (corresponding to $E_p \approx 66$ eV, the maximum energy used in ARPES), we cannot validate the free-electron assumption for the final state for sodium. Thus the energy band obtained from the ARPES data analyzed on the free-electron assumption [28] should not be compared with our E_p directly but with "the virtual energy band" E_p^{vir} , defined by [2]

$$E_p^{\text{vir}} \equiv E_p - \text{Re}\Sigma(\mathbf{p} + \mathbf{K}_{[110]}, E_{\mathbf{p}+\mathbf{K}_{[110]}}), \quad (17)$$

with $\mathbf{K}_{[110]}$ the reciprocal-lattice vector in the direction [110]. As is seen in Fig. 3, though the result in Ref. [2] (the dot-dashed curve) is fairly good, our result is in perfect agreement with experiment. Implications of this result will be discussed in detail elsewhere, together with a similar analysis on aluminum.

To sum up, we have proposed a useful functional form for the vertex function incorporating the Ward identity and the accurate information on static quantities provided by

quantum Monte Carlo simulations. By implementing the self-consistent calculation of the self-energy with the vertex function, we conclude that the occupied bandwidth of sodium is slightly widened.

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