Improved local-field corrections to the G_0W approximation in jellium: Importance of consistency relations

M. Hindgren and C.-O. Almbladh

Department of Theoretical Physics, Lund University, Sölvegatan 14 A, S-223 62 Lund, Sweden

(Received 11 June 1997)

We study the effects of local vertex corrections to the self-energy of the electron gas. We find that a vertex derived from time-dependent density-functional theory can give accurate self-energies, provided, however, a proper decay at large momentum transfer (large q) is built into the vertex function. (The local-density approximation for the vertex fails badly.) Total energies are calculated from the Galitskii-Migdal formula, and it is shown that a proper large-q behavior results in a close consistency between the chemical potentials derived from these energies and those obtained directly from the self-energy. We show that this internal consistency depends critically on including the same vertex correction in both the self-energy and the screening function. In addition the total energies become almost as accurate as those from elaborate Monte Carlo calculations. This as well as previous works show that self-energy corrections are important for properly describing electron propagation at energies around and above the plasmon energy. For easy use in calculations of photoemission and x-ray extended fine structure spectra, we parametrize our calculated self-energies in terms of a simple analytical expression. [S0163-1829(97)03040-3]

I. INTRODUCTION

The dynamically screened-exchange or GW approximation[1] has emerged as a successful tool for obtaining quasiparticle bands in real solids. As usually practiced, the self-consistency requirement on the self-energy Σ is relaxed and typical calculations involve a suitably chosen independent-particle Green's function G_0 (the G_0W approximation). In attempts to go beyond the GW_0A, one has added vertex corrections derived using mean-field arguments or time-dependent density-functional theory (TDDFT).[2–7] However, these efforts have shown little effect on the quasiparticle bands.

A closer examination of the G_0WA shows that, although it usually gives a good description of the relative positions of the occupied bands, it also gives a rather large absolute error. For the occupied states, the errors in quasiparticle energies are similar in magnitude. When we move from the Fermi energy up to high energies, however, the self-energy varies from relatively large negative values up to zero. Consequently, absolute errors will distort the relative positions of the higher bands.

In this paper, we will study mean-field based vertex approximations using the homogeneous electron gas as a test system. We will demonstrate the severe shortcomings of the vertex corrections derived from the time-dependent local-density approximation (TDLDA). We trace this failure to the wavelength independence of the corresponding local-field correction. Including, however, a Hubbard-like decay at large momentum transfer (large q=$|\mathbf{q}|$), we obtain significant improvements beyond the G_0WA. In particular, the Fermi-surface value is greatly improved. In order to investigate the internal consistency of our approach we also compute total energies from the Galitskii-Migdal formula.[8] In this way, we can compare chemical potentials derived from the total energy and from the self-energy at the Fermi sur-

face. As we will show, the TDDFT approach greatly improves the consistency between the total energy and the self-energy as well as their absolute values.

The self-energy for the homogeneous system has some interest on its own right as a starting point for local approximations to Σ in, say, calculations of x-ray extended fine structure (EXAFS) and electron spectroscopies. In order to facilitate such a use of our data we provide simple analytical fits.

In Sec. II we give a theoretical background and discuss different ways of obtaining approximate vertex functions. Results and parametrization are given in Sec. III, and in Sec. IV, finally, we give some concluding remarks.

II. THEORETICAL BACKGROUND

A. The electron self-energy

In this section we summarize some key formulas in order to establish our notation. For a general overview we refer to the work by Hedin and Lundqvist.[9]

The self-energy Σ may be defined from the equation of motion for the Green's function G as

$$\left[\epsilon + \frac{\nabla^2}{2} - V_C \right] G(\epsilon) = 1 + \Sigma(\epsilon) G(\epsilon). \qquad (1)$$

Here V_C is the total Coulomb potential from the electron ground-state density (V_H) and from external sources (w), and we use atomic units with energies in Hartrees. Specializing to a homogeneous electron gas, $V_C = 0$ in equilibrium. The self-energy can be written explicitly as

$$\Sigma(k) = i \int \frac{d^4q}{(2\pi)^4} G(k-q) W(q) \Lambda(k,q). \qquad (2)$$

Here, the dynamically screened interaction $W = \epsilon^{-1} v$, ϵ is the dielectric screening function, and v is the Coulomb interaction. We use the simplified notation $k = (\mathbf{k}, \epsilon)$ and $\mathrm{k} = |\mathbf{k}|$. The vertex function Λ gives the (linear) response in Σ when we break the translational invariance by a nonzero $V_C(q)$,

$$\Lambda(k,q) = 1 + \frac{\delta\Sigma(k,q)}{\delta V_C(q)}. \tag{3}$$

Also the dielectric function ϵ can be expressed solely in the Green's function and the same vertex as above. It is customary to introduce an irreducible polarization P by the relation

$$\epsilon(q) = 1 - v(q) P(q), \tag{4}$$

where

$$P(q) = -2i \int \frac{d^4 k}{(2\pi)^4} G(k) G(k-q) \Lambda(k,q). \tag{5}$$

As is well known, in perturbation theory Σ will inherit the Fermi surface of the independent-electron propagator G_0.[10,11] Consistency therefore requires that we add a one body potential to the noninteracting system so as to keep the Fermi surface unchanged. In a homogeneous systems, this potential is simply a constant,

$$\Delta = \mu_{\mathrm{xc}} = \Sigma(k_F, \mu), \tag{6}$$

where μ and μ_{xc} are the chemical potential and its exchange-correlation part, and where k_F is the Fermi momentum. From the equation of motion [Eq. (1)] we readily find

$$G(\mathrm{k}, \epsilon) = [\epsilon - \epsilon_{\mathrm{k}}^0 - \Sigma(\mathrm{k}, \epsilon)]^{-1}, \tag{7}$$

$$G_0(\mathrm{k}, \epsilon) = [\epsilon - \epsilon_{\mathrm{k}}^0 - \Delta + i\delta\,\mathrm{sgn}(\epsilon - \mu)]^{-1}, \tag{8}$$

(δ being a positive infinitesimal and $\epsilon_{\mathrm{k}}^0 = \mathrm{k}^2/2$), and a Dyson equation connecting the two Green's functions,

$$G(k) = G_0(k) + G_0(k) [\Sigma(k) - \Delta] G(k). \tag{9}$$

The quasiparticle energies ϵ_{k} are obtained from

$$\epsilon_{\mathrm{k}} = \epsilon_{\mathrm{k}}^0 + \mathrm{Re}\,\Sigma(\mathrm{k}, \epsilon_{\mathrm{k}}). \tag{10}$$

B. Approximation for the vertex function

The GW approximation consists of approximating the vertex in Eq. (3) by unity. On this level, the approximation is conserving in the sense of Baym and Kadanoff,[12,13] which, among other things, implies mutual consistency between the total energy and the Fermi-surface value of Σ. In the $G_0 WA$ we furthermore replace all propagators by their independent-electron counterparts (G_0). Thus,

$$\Sigma(k) = i \int \frac{d^4 q}{(2\pi)^4} G_0(k-q) W(q). \tag{11}$$

and P is approximated by the independent-electron polarizability

$$P_0(q) = -2i \int \frac{d^4 k}{(2\pi)^4} G_0(k) G_0(k-q). \tag{12}$$

The energy shift Δ in G_0 [Eq. (8)] gives merely a shift in the frequency variable of Σ, $\epsilon \to \epsilon - \Delta$.

One way to go beyond the $G_0 WA$ is to imagine that the interacting electrons respond as free electrons to an effective field V_{eff}. As far as static perturbations are concerned, density-functional theory[14,15] then, in principle, gives the exact results. In the case of time-dependent phenomena, this way of looking at the problem has been successfully used by Singwi, Sjölander, and collaborators[16,17] for modeling the dielectric function. Similar ideas have been applied to the problem of core electrons by Minnhagen.[18] Also Mahan and Sernelius[6] and Del Sole et al.[7] extend the GW approximation along these lines. We thus calculate the response of our system in a one-particle manner using the effective potential,

$$\delta V_{\mathrm{eff}}(q) = \delta V_C(q) + \delta v_{\mathrm{xc}}(q), \tag{13}$$

where we identify the exchange-correlation part v_{xc} with the density-functional ground-state potential. Comparing with Eq. (3) we see that the change in the self-energy has been replaced by the corresponding change in v_{xc}. This leads to approximations to Λ and W given by

$$\Lambda(q) = \frac{\delta V_{\mathrm{eff}}(q)}{\delta V_C(q)} = \frac{1}{1 - P_0(q) K_{\mathrm{xc}}(q)}, \tag{14}$$

$$W(q) = v(q) \frac{\delta V_C(q)}{\delta w(q)} = \frac{v(q)[1 - K_{\mathrm{xc}}(q) P_0(q)]}{1 - P_0(q)[v(q) + K_{\mathrm{xc}}(q)]}. \tag{15}$$

Here, K_{xc} is a functional derivative of v_{xc} with respect to the density,

$$K_{\mathrm{xc}}(q) \equiv \frac{\delta v_{\mathrm{xc}}(q)}{\delta n(q)}. \tag{16}$$

If the Green's function in Eq. (2) is again approximated by the independent-electron Green's function G_0, we obtain

$$\Sigma(k) = i \int \frac{d^4 q}{(2\pi)^4} G_0(k-q) \widetilde{W}(q), \tag{17}$$

where the effective screened interaction $\widetilde{W}$ is given by

$$\widetilde{W}(q) = W(q) \Lambda(q) = \frac{v(q)}{1 - P_0(q)[v(q) + K_{\mathrm{xc}}(q)]}. \tag{18}$$

The basic building block in the present TDDFT approximation is the function $K_{\mathrm{xc}}(q)$. Unfortunately, it is accurately known only in the limit of spatially slowly varying densities appropriate to the LDA. Of course, even if we knew K_{xc} exactly our approach is still approximate because the state

and energy dependent self-energy has been replaced by a local potential when deriving Λ.

It should be noted that our effective vertex accounts, in some average way, for both self-consistency corrections arising from the difference between G and G_0 as well as proper vertex corrections. If we would solve the GW equations self-consistently, as has been done by Holm and von Barth,[19] one encounters subtle problems which are not yet fully understood. The problems originate in the different levels of responses in conserving theories.[13] The self-energy and thus the screening function(s) to be used in constructing it emerges as a first-order derivative of an underlying Φ functional with respect to G. The actual response function of the theory is defined as a second-order derivative and is, in general, different for approximate functionals. In the case of the GW approximation, this latter response function ("time-dependent GW approximation") is only known in the high-density limit.[20] Particle conservation requires that the vertex must be a functional derivative of Σ (Refs. 12 and 13) as in Eq. (3). In GW theory the appropriate vertex is produced when the total energy is differentiated twice to form the correct response function, *but not in the intermediate step which defines Σ and P*. Holm and von Barth indeed detect a large violation of the f-sum rule. Approximations like the present one with independent-electron Green's functions have no Σ entering in the calculation of W. They are consequently compatible with having no vertex corrections at all (the G_0WA) as well as with having vertices depending only on the momentum transfer q.

In works on the dielectric function, the effective vertex is usually expressed in a "local-field factor" $f(q)$. In our density-functional description, we have

$$f(q) = -\frac{1}{v(q)} K_{xc}(q). \tag{19}$$

It is generally accepted that this local-field factor should tend to a constant of the order unity for large $q = |\mathbf{q}|$ and that it should level off from its quadratic low-q behavior around $q = 2k_F$. In the strict static limit of the density-response function, Niklasson[21] has shown that $f(q)$ tends to a limit between 1/3 and 2/3 for high q. Recent quantum–Monte Carlo calculations give $f(q)$ for intermediate q.[22]

In the local-density approximation (TDLDA), K_{xc} is replaced by its low-q limit $d\mu_{xc}/dn$, and $f(q)$ tends to infinity as q^2 for large q. The TDLDA has been successfully applied to atoms,[23] and most calculations in solids employ the same approximation. While the TDLDA certainly is correct for slowly varying static perturbations, it gives a very unphysical local-field factor for higher q. In order to investigate the importance of the high-q behavior, we study also time-dependent density-functional approximations which interpolate between the LDA values for low-q to a high-q behavior with a $f(\infty)$ in the range 1/2–1:

$$K_{xc}(q) = \frac{K_{xc}(0)}{1 + (q/\alpha)^2}. \tag{20}$$

A similar *Ansatz* has been used by Shirley[24] for estimating the first vertex diagram. We fix α to have a given value of $f(\infty)$. In our calculations, $K_{xc}(0)$ was obtained from data by

TABLE I. Relation between α and $f(\infty)$ [Eq. (20)].

r_s	α/k_F [$f(\infty)=\frac{1}{2}$]	α/k_F [$f(\infty)=1$]
2	2.73	1.93
4	2.67	1.89
6	2.62	1.85

Ceperley and Alder[25] as parametrized by Vosko *et al.*[26] In Table I we give the mapping between $f(\infty)$ and α. The sensitivity of the final results on different choices of $f(\infty)$ will be discussed in the next section. It is also of interest to know how sensitive the results are to the detailed shape of K_{xc}. To this end, we also do calculations with local-field factors suggested by Hubbard,[27] Vashishta and Singwi,[17] and by Geldart and Vosko.[28] They all give very similar results, as does the interpolation scheme suggested here.

So far we have tacitly assumed that the same local-field correction should be applied to both the screening and directly in Σ. This seems most natural because in the exact expressions it is the same vertex that occurs in both places. However, different procedures have been used in the past in order to explain the band narrowing in the heavy alkali metals. In order to shed light on the usefulness of such schemes we also perform calculations with local-field effects only in the screening or only in the self-energy.

C. Ground-state energy

As shown by Galitskii and Migdal[8] (GM) the ground-state energy can be expressed in terms of the one-particle Green's function of the system. Since we are considering the total energy, which is a thermodynamic property, it is natural to use the finite temperature formalism in its $T=0$ limit. This method is also computationally more efficient. The GM formula was first applied to the electron gas by Lundqvist and Samathiyakatanit.[29] (No other extended system has, to our knowledge, been treated.)

According to GM, the grand potential Ω for a homogeneous system can be written as

$$\Omega = \langle \hat{T} - \mu\hat{N} + \hat{U}\rangle = 2\sum_{\mathbf{k}} (\epsilon_{\mathbf{k}}^0 - \mu)n_{\mathbf{k}} + \frac{1}{2}\text{Tr}\widetilde{\Sigma}\mathcal{G}, \tag{21}$$

where $\hat{T}$, $\hat{N}$, $\hat{U}$ are the operators for kinetic energy, particle number, and interaction energy, respectively. In Eq. (21) we have introduced the Matsubara[30] counterparts to the Green's function and self-energy,

$$\mathcal{G}(\mathbf{k},\epsilon) = G(\mathbf{k},i\epsilon+\mu), \tag{22}$$

$$\widetilde{\Sigma}(\mathbf{k},\epsilon) = \Sigma(\mathbf{k},i\epsilon+\mu), \tag{23}$$

and $n_{\mathbf{k}}$ are the occupation numbers. The symbol Tr is short for

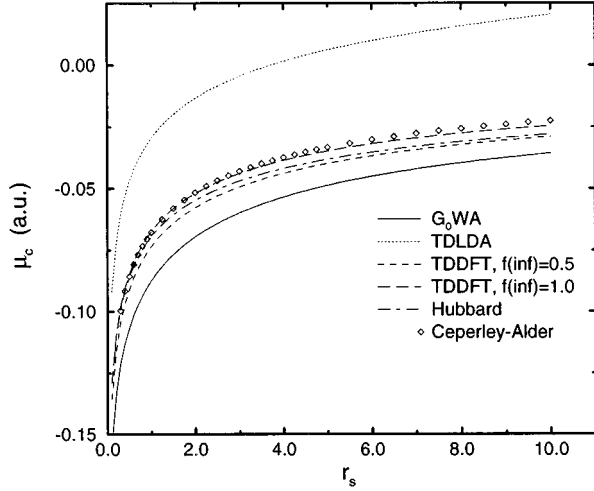$$2\sum_{\mathbf{k}} \int \frac{d\epsilon}{2\pi}e^{i\delta\epsilon},$$

FIG. 1. The correlation potential (μ_c) for an unpolarized electron gas from different approximate self-energies and from quantum–Monte Carlo calculations by Ceperley and Alder.

FIG. 2. The correlation energy per particle calculated from Eq. (24) with $\Sigma(k, r_s)$ calculated from Eq. (11) (G_0WA) and from Eq. (17) (TDDFT) are compared with the values by Ceperley and Alder and with the corresponding RPA values.

where the limit $\delta \to 0^+$ should be taken at the end of the calculation.

The nontrivial part of Ω is the correlation energy, or rather the correlation energy per particle ϵ_c. We thus subtract the exchange energy and independent-electron kinetic energy and divide by the particle number N. This gives

$$\epsilon_c = \frac{1}{N}\left[2\sum_{\mathbf{k}} \left(\epsilon_{\mathbf{k}}^0 + \frac{1}{2}\Sigma_x(k) \right)\Delta n_{\mathbf{k}} + \frac{1}{2}\,\mathrm{Tr}\widetilde{\Sigma}_c \mathcal{G}\right]. \quad (24)$$

Here $\Delta n_{\mathbf{k}}$ is the difference between occupation numbers with and without interaction, Σ_x is the Hartree-Fock self-energy, and $\widetilde{\Sigma}_c = \widetilde{\Sigma} - \Sigma_x$. Theoretically, it is not clear if one should use the particle number from $\mathcal{G}$ or from $\mathcal{G}_0$ for obtaining ϵ_c. However, we find that the particle number from $\mathcal{G}$ is conserved to within 0.01% in the entire range $r_s \leqslant 6$.

III. RESULTS

A. Chemical potential and total energy

In order to assess the merits of different local-field approximations we need information about the self-energy obtained by other means. Generally, little is known about Σ beyond the G_0WA level except at the Fermi surface, where is should yield the exchange-correlation part μ_{xc} of the chemical potential [cf. Eq. (6)]. The latter quantity is rather well known from quantum Monte Carlo calculations by Ceperley and Alder.[25] In Fig. 1 we compare the correlation part of the chemical potential $\mu_c = \widetilde{\Sigma}_c(k_F, 0)$ in different approximations with results derived from the Ceperley-Alder data by Vosko et al.[26] We notice that the G_0WA overestimates the magnitude of μ_c by as much as 40% in the metallic range, and that TDLDA [$K_{xc}(q) = K_{xc}(0)$] is way above and has even the incorrect sign for r_s larger than 4.

In the case of G_0WA, one can actually show that the Fermi-surface value should equal the value obtained from the random phase approximation (RPA) dielectric function integrated over the interaction strength.[31] (This correspondence is fulfilled to 0.01% or better in our numerical data.) It
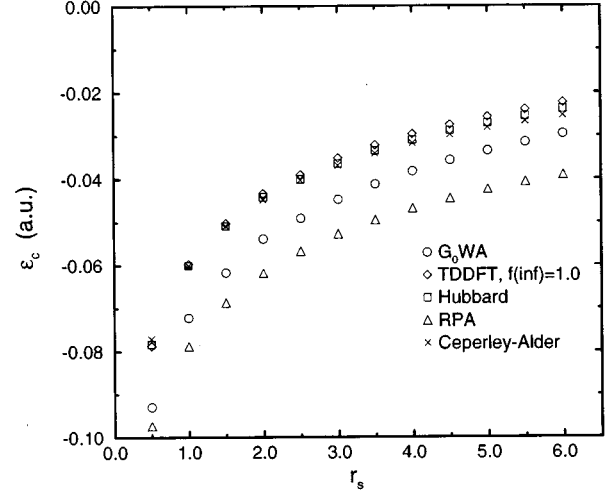
is well known that the RPA overestimates the correlation energies, and the G_0WA inherits this deficiency. In calculations of occupied-state energies, though, the self-energy is rather constant, and this relatively large but constant error has little effect on the relative positions of occupied bands.

The very bad behavior of the TDLDA can be understood as follows. The self-energy depends on the effective interaction in Eq. (18), for all q. The spectral function for the effective interaction is

$$-\,\mathrm{Im}\;\widetilde{W}(q)\mathrm{sgn}(\omega) = \frac{[1 - f(q)](v(q))^2 \pi S_0(q)}{|1 - [1 - f(q)]P_0(q)v(q)|^2}. \quad (25)$$

(S_0 is the independent-electron structure factor.) Because $f(\mathrm{q})$ increases as q^2 in the TDLDA, the effective interaction will have a negative spectral function at higher q. The spectral function has a plasmon part arising from the zeros of the denominator, and a particle-hole part arising from the numerator. The resulting self-energy still has a non-negative spectral function, but its electron-hole part from the electron-hole part of $\widetilde{W}$ is negative at higher momenta. This unphysical behavior of the spectral function of $\widetilde{W}(q)$ is the likely reason why the TDLDA fails.

Proceeding to the local-field corrections by Hubbard,[27] Vashishta and Singwi,[17] and the TDDFT interpolation formula of the previous section [Eq. (20)] with $f(\infty) = 1/2$, we notice that they all give very similar results and correct roughly 2/3 of the G_0WA error. If we stretch the interpolation to allow $f(\infty) = 1$, the resulting Fermi-surface values agree with the Ceperley-Alder data within 1–2 %. This very good agreement is of course much better than expected from such a simple approximation. Being interested in quasiparticle energies at all momenta, we feel it is justified to use this value of α to calculate the self-energy also away from the Fermi surface.

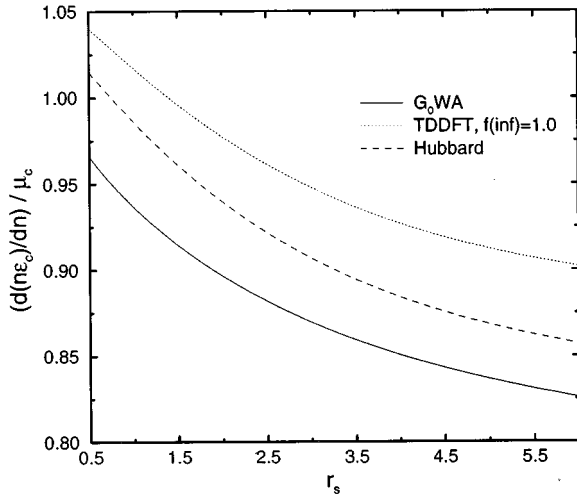In Fig. 2 we show the correlation energy per particle in

FIG. 3. The violation of the consistency relation in Eq. (26) in different approximations.

FIG. 4. The chemical potential with $f(\infty)=1$. The results when local fields are included only in the screening and only in Σ are compared with the values by Ceperley and Alder.

different approximations. Again we compare with Ceperley-Alder data as compiled by Vosko *et al.*

We notice that the energies from the G_0WA are approximately midway between the RPA values, which are too deep, and the Ceperley-Alder values. This confirms the conclusion by Lundqvist and Samathiyakatanit[29] that already this first approximation represents a considerable improvement. The various local-field corrections with exception of the TDLDA give similar results and they are close to the Ceperley-Alder data.

In an exact theory, the self-energy is related to the correlation energy by

$$\Sigma_c(k_F,\mu) = \frac{d}{dn}(n\epsilon_c(n)) \qquad (26)$$

($\Sigma_c = \Sigma - \Sigma_x$). This consistency relation is violated in the G_0WA. By adding local-field corrections, both the Fermi-surface value of Σ and the correlation energy approach the Ceperley-Alder values [which by construction fulfill $\mu_c = d(n\epsilon_c)/dn$]. Thus the violation is greatly reduced by the local-field corrections. The violation of the consistency relation in Eq. (26) in different approximations is plotted in Fig. 3.

As mentioned in the previous section, consistency between the Fermi-surface value of Σ and the total energy is guaranteed in any conserving approximation. Thus, it is obeyed in the first self-consistent solution to the GW functional by Holm and von Barth.[19] Their correlation energies and chemical potentials are very close to the ones obtained with our interpolation scheme here. Thus, the local-field corrections have largely removed the self-consistency errors inherent in the G_0WA. That this is at all possible gives some credibility to our approach.

Let us finally discuss approximations with local fields in only the screening function or only in Σ. In Fig. 4 we show results for the chemical potential with $f(\infty)=1$.

When local fields are included only in the screening function, we see that μ_c drops way below the already too deep G_0WA values. If, on the other hand, the local fields are in-
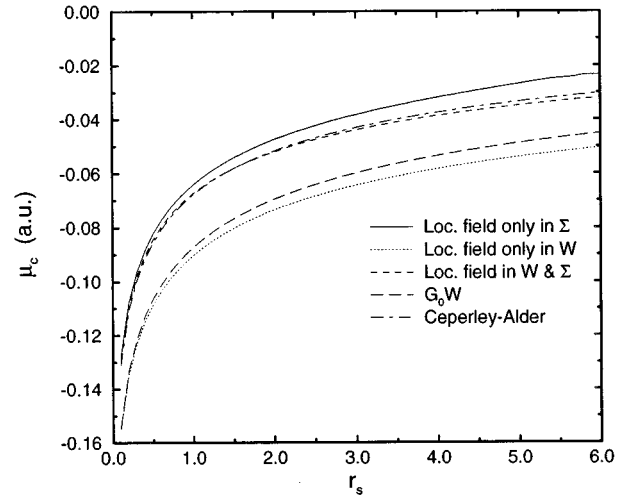
cluded in Σ but not in the screening function, μ_c is pushed above the Ceperley-Alder results. Looking at the total energies (Fig. 5) we see the same trends but somewhat less pronounced. Thus, the correlation energy drops below the G_0WA results when local fields are included only in the screening, and it is pushed above the Ceperley-Alder values with local fields only in Σ. The other local-field approximations (Hubbard, etc.) give similar results. It is clear that by including local-field effects only in the screening or only in Σ we destroy the consistency between the chemical potential and the total energy and also the quality of the G_0WA results. Our findings support the conclusions by Mahan and Sernelius[6] concerning the inadequacy of such approximations.

B. Parametrization of quasiparticle dispersions

The electron-gas quasiparticle energies within the G_0WA were obtained long ago by Hedin and Lundqvist,[32,33] and calculations with local-field corrections, like the present
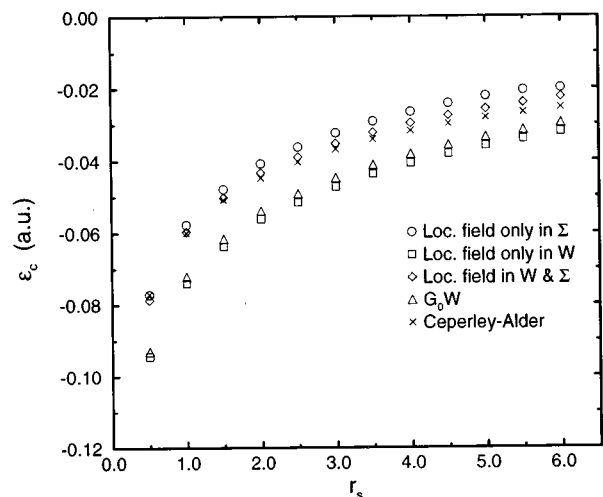

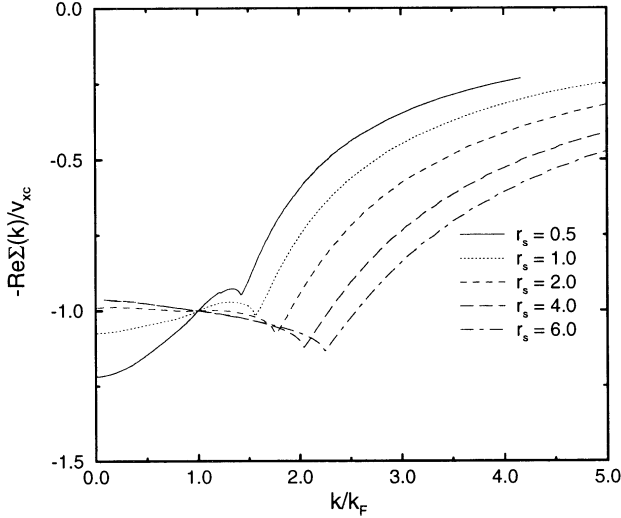FIG. 5. The correlation energy with $f(\infty)=1$ as in Fig. 4.

FIG. 6. The k dependence of Re $\Sigma(\mathrm{k}, r_s)$ from Eq. (11) (G_0WA).

ones, were obtained by Mahan and Sernelius,[6] although they only present changes in the bandwidths. Our results can be used to construct local approximations[33,34] to Σ which are useful in calculations of, for example, electron energy loss or photoelectron propagation. It may therefore be of some interest to have a compilation of results with local-field corrections in a convenient parametrized form. We thus calculate Re $\Sigma(\mathrm{k})=$Re $\Sigma(\mathrm{k}, \epsilon_k)$ at the quasiparticle energy ϵ_k [Eq. (10)]. Results at different densities are compared with those of the G_0WA in Figs. 6 and 7. The dispersions from the G_0WA and from TDDFT are very similar in shape, in agreement with previous findings.[6]

At higher energies where plasmon losses become possible, roughly a plasmon energy above the Fermi energy, the dispersion corrections become more pronounced. Photoelectron energies typically fall in this energy region, and the self-energy corrections are quite important here. In the case of the quasiparticle damping, again the straight G_0WA are similar but somewhat larger than those of TDDFT.
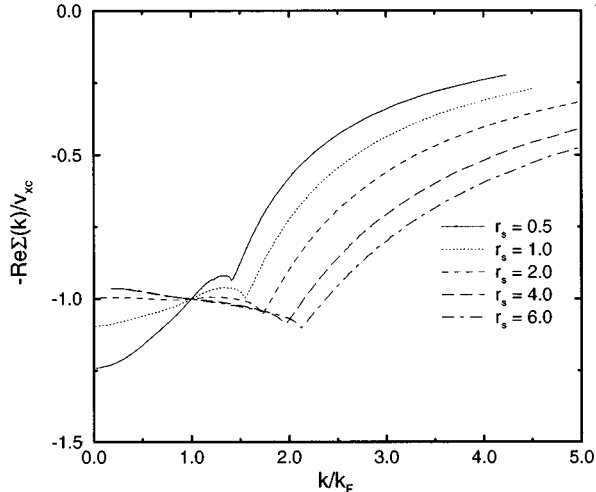

FIG. 7. The k dependence of Re $\Sigma(\mathrm{k}, r_s)$ from Eq. (17) (TDDFT) with $f(\infty)=1$.

The quasiparticle strength $Z=[1-(\partial\Sigma/\partial\epsilon)]^{-1}$ with and without local-field effects are also very similar. Below the threshold for plasmon excitation, Z is of the order of 0.6–0.8, and it rapidly approaches unity above the threshold.

The results from the calculation of Re $\Sigma(k)$ have been parametrized in terms of simple functions of momentum and density. Because the ground-state potential is much better known than the self-energy, it is natural to parametrize the quantity

$$F(\mathrm{k}, r_s) = \frac{\mathrm{Re}\ \Sigma(\mathrm{k}, r_s)}{v_{\mathrm{xc}}(r_s)}, \qquad (27)$$

rather than Σ itself. The function F is calculated in the G_0WA from Eq. (11) and in the TDDFT from Eq. (17) with $v_{\mathrm{xc}}=\Sigma(k_F, \mu)$ for consistency. The calculated values of F are in both cases parametrized and the explicit expressions for the parametrizations of F are given in the Appendix. The parametrizations of the function F are constructed in such a way that the approximate Re $\Sigma(k)$ obtained from these functions have the same main analytical properties as the exact electron self-energy. The latter has two main features:

$$\lim_{\mathrm{k}\to\infty} \mathrm{Re}\ \Sigma(\mathrm{k}) \propto \frac{1}{\mathrm{k}},$$

$$\lim_{\mathrm{k}\to 0} \frac{\partial\ \mathrm{Re}\ \Sigma(\mathrm{k})}{\partial\mathrm{k}} = 0.$$

In both the G_0WA and in TDDFT the real part of $\Sigma(\mathrm{k})$ has a cusp at $\mathrm{k}=\mathrm{k}_c$, where plasmon excitations become possible. This is a consequence of the fact that, in our approximation, the plasmons are sharp excitations until they hit the particle-hole continuum. In the exact dielectric function the plasmons are broadened and the cusp in Re $\Sigma(\mathrm{k})$ is smoothed. We have therefore introduced an extra parameter γ in the parametrizations of F which simulates this broadening. The parameter only affects the behavior of the parametrization of Re $\Sigma(\mathrm{k})$ in the vicinity of $\mathrm{k}=\mathrm{k}_c$ and $\gamma=0$ reproduces the calculated results. Both parametrizations for Re $\Sigma(\mathrm{k})$ reproduces the calculated values for $0.3 \leqslant r_s \leqslant 6$ and $\mathrm{k} < 2k_F$ to within 5%.

IV. CONCLUSIONS

In this paper we have scrutinized commonly used mean-field-type vertex corrections using as a guiding principle the consistency between the total energy and the chemical potential. We have shown that rather simple local-field approximations derived from time-dependent density-functional theory can be used to systematically improve the absolute values of the self-energy. In particular, the rather large error in the correlation potential at the Fermi surface can be almost entirely eliminated. In doing so, the total energy and the chemical potential become approximately consistent and rather close to quantum Monte Carlo results and to those from a self-consistent solution to the GW problem.

We have also been able to isolate some severe problems with approximation schemes used in the past. Thus, we have

found that the time-dependent LDA gives bad results and that it is essential that the local-field reflects density changes in a region of the order of the screening length in the system. We have also demonstrated that local-field corrections should be applied consistently to both the screening function and to Σ itself.

Like previous workers, we find little effects on occupied states on a relative energy scale. All vertex corrections considered here are local, i.e., they depend only on the momentum transfer q and not on the momenta and energies of the colliding electrons. A common theme from many investigations is that vertex approximations of this kind have little effect on the quasiparticles around and below the Fermi energy.[6,5,7,35] In the case of band gaps in semiconductors, it is known that it is primarily the *nonlocality* of the self-energy that is of importance, and not so much its energy dependence. Vertex approximations depending only on q are obtained from a *local* approximation to Σ. Thus, it seems conceivable that approximations based on a nonlocal *ansatz* are to be preferred. The consistency requirements discussed in the present work will be useful in deriving such more advanced approximations. Finally, we provide simple fits to quasiparticle energies in the hope that they may be useful in approximate calculations of spectra involving electrons at higher energies, such as photoemission and EXAFS spectra.

ACKNOWLEDGMENTS

APPENDIX: PARAMETRIZATION

The function F discussed in Sec. III B is given by

$$F(k,\gamma,r_s)=c_0 A(K)+\frac{c_2 B(K)}{2\pi\sqrt{1+c_3}}[1+[B(K)]^3]$$

$$\times \mathrm{Im}\ln z_2 + C(K)\mathrm{Im}\ln z_1, \quad (A1)$$

where

$$K=\frac{k}{c_4}, \quad (A2)$$

$$A(K)=\mathrm{Re}\ln z_1 \frac{1-K^2}{2\pi K}\mathrm{Im}[\ln z_1 - \ln z_2]+1, \quad (A3)$$

$$B(K)=\sqrt{\frac{c_1+1}{c_1+K^2}}, \quad (A4)$$

$$C(K)=\frac{c_2}{\pi\sqrt{1+c_3 K^2}}, \quad (A5)$$

$$z_1=-z_2^*=\frac{K-1}{K+1}+i\frac{4\gamma K^4}{(1+K^4)^2}. \quad (A6)$$

TABLE II. $G_0 WA$ constants.

m/n	0	1	2	3
			c_{mn}	
0	0.170073	-0.461614	0.766573	-0.0436796
1	3.014	-1.20923	4.03085	-2.43659
2	1.01252	-0.44149	1.13575	0
3	0.735628	0.548797	0.817027	0
4	3.00073	-0.913005	-0.873964	1.12073

The parameters $c_0,\ldots,c_4$ are all functions of r_s and are given by

$$c_0(r_s)=\left[\frac{c_{00}r_s}{\sqrt{1+r_s^2}}+\frac{\sqrt{r_s}(c_{01}+c_{02}\sqrt{r_s}+c_{03}r_s)}{1+r_s^4}\right]\theta(c_0), \quad (A7)$$

$$c_1(r_s)=\left[\frac{c_{10}r_s}{\sqrt{1+r_s^2}}+\frac{r_s(c_{11}+c_{12}r_s+c_{13}r_s^2)}{1+r_s^4}\right]\theta(c_1-10^{-6}), \quad (A8)$$

$$c_2(r_s)=c_{20}+\frac{c_{21}}{1+r_s}+\frac{c_{22}}{(1+r_s)^2}, \quad (A9)$$

$$c_3(r_s)=c_{32}[e^{-c_{30}r_s}+e^{-c_{31}r_s^2}], \quad (A10)$$

$$c_4(r_s)=c_{40}r_s^{[(c_{41}+c_{42}r_s)/(1+c_{43}r_s)]}. \quad (A11)$$

The constants c_{mn} are given in Tables II and III.
Note that the condition

$$F(k_F(r_s),\gamma,r_s)=1, \quad (A12)$$

from Eq. (6) is not exactly fulfilled by this parametrization. If this property is desired, the expression for F in Eq. (A1) should be divided by $F(k_F)$. If this is done, the agreement with the calculated values of F is slightly worse but still within the accuracy mentioned in Sec. III B. For those interested, the computer code for this parametrization is available via anonymous ftp at *ftp.teorfys.lu.se.*

TABLE III. TDDFT constants.

m/n	0	1	2	3
			c_{mn}	
0	0.13405	-0.1245	0.0124766	0.384274
1	3.68646	-2.08264	5.10236	-3.87509
2	1.00252	-0.367488	1.10035	0
3	0.775477	0.516925	0.893986	0
4	2.96853	-0.910738	-1.2975	1.58913

[1] L. Hedin, Phys. Rev. **139**, A796 (1965).

[2] A. W. Overhauser, Phys. Rev. B **3**, 1888 (1971).

[3] A. K. Rajagopal, Phys. Rev. B **17**, 2980 (1978).

[4] M. S. Hybertsen and S. G. Louie, Phys. Rev. B **34**, 5390 (1986).

[5] C. Petrillo and F. Sacchetti, Phys. Rev. B **38**, 3834 (1988).

[6] G. D. Mahan and B. E. Sernelius, Phys. Rev. Lett. **62**, 2718 (1989).

[7] R. Del Sole, L. Reining, and R. W. Godby, Phys. Rev. B **49**, 8024 (1994).

[8] V. M. Galitskii and A. B. Migdal, Zh. Eksp. Teor. Fiz. **34**, 139 (1958) [Sov. Phys. JETP **7**, 96 (1958)].

[9] L. Hedin and S. Lundqvist, in *Solid State Physics: Advances in Research and Applications*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1969), Vol. 23, p. 1.

[10] W. Kohn and J. M. Luttinger, Phys. Rev. **118**, 41 (1960).

[11] P. Nozières, *Theory of Interacting Fermi Systems* (Benjamin, New York, 1964).

[12] G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 286 (1961).

[13] G. Baym, Phys. Rev. **127**, 1391 (1962).

[14] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).

[15] W. Kohn and L. J. Sham, Phys. Rev. **140**, 1133 (1965).

[16] K. S. Singwi, A. Sjölander, M. P. Tosi, and R. H. Land, Phys. Rev. B **1**, 1044 (1970).

[17] P. Vashishta and K. S. Singwi, Phys. Rev. B **6**, 566 (1980).

[18] P. Minnhagen, J. Phys. C **7**, 2464 (1977).

[19] B. Holm and U. von Barth, Phys. Rev. B (to be published December 15, 1997).

[20] D. C. Langreth and S. H. Vosko, Phys. Rev. Lett. **59**, 497 (1987).

[21] G. Niklasson, Phys. Rev. B **10**, 3052 (1974).

[22] C. Bowen, G. Sugiyama, and B. J. Alder, Phys. Rev. B **50**, 14 838 (1994).

[23] A. Zangwill and P. Soven, Phys. Rev. A **21**, 1561 (1980).

[24] E. L. Shirley, Phys. Rev. B **54**, 7758 (1996).

[25] D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. **45**, 566 (1980).

[26] S. H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. **58**, 1200 (1980).

[27] J. Hubbard, Proc. R. Soc. London, Ser. A **243**, 336 (1957).

[28] D. J. W. Geldart and S. H. Vosko, Can. J. Phys. **44**, 2137 (1966).

[29] B. I. Lundqvist and V. Samathiyakatanit, Phys. Kondens. Mater. **9**, 231 (1969).

[30] T. Matsubara, Prog. Theor. Phys. **14**, 351 (1955).

[31] U. von Barth (unpublished).

[32] B. I. Lundqvist, Phys. Status Solidi **32**, 273 (1969).

[33] L. Hedin and B. I. Lundqvist, J. Phys. C **4**, 2064 (1971).

[34] L. J. Sham and W. Kohn, Phys. Rev. **145**, 561 (1966).

[35] G. D. Mahan, Mod. Phys. Lett. **7**, 13 (1993).