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Phys. Rev. B **98**, 115125 — Published 14 September 2018

DOI: 10.1103/PhysRevB.98.115125

Coulomb-hole and screened-exchange in the electron-self energy at finite temperature

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(Dated: August 27, 2018)

We present a finite temperature generalization of the COHSEX approximation to the quasi-particle electron self-energy, with explicit comparisons of the static and dynamic screened exchange (SEX) and Coulomb hole (COH) contributions for the homogeneous electron gas. Consistent with the zero-temperature behavior, we show that the static SEX approximation agrees well with the fully dynamic SEX at all temperatures and densities. In contrast, dynamic corrections to the COH approximation are always significant, especially for high energy unoccupied states. Notably the COHSEX quasi-particle self-energy is complex-valued at finite-T even at the Fermi level.

I. INTRODUCTION

Recently there has been considerable interest in properties of matter at finite-temperatures (FT) and extreme conditions.[1–3] Such properties are often treated using the FT generalization of density functional theory (DFT), with an appropriate FT exchange-correlation functional.[4–7] However, many properties, such as band-gaps and optical spectra require many-body corrections for an accurate treatment. Consequently a more detailed treatment of exchange and correlation effects beyond DFT are often needed.[8]

Formally, such effects can be described in terms of the one-electron Green's function G, which satisfies a Dyson equation $G = G_0 + G_0\Sigma G$, which is also applicable at finite T for either the Matsubara or retarded Green's functions. Here G_0 is the one-electron Green's function, and Σ the one-electron self-energy which accounts for many body exchange and correlation effects due to electron-electron interactions v. In principle, Σ can be calculated using many-body perturbation theory with an expansion in powers of v. However, this procedure converges poorly, and a better strategy is to expand in powers of the screened Coulomb interaction $W(q,\omega) = \epsilon^{-1}(q,\omega)v_q$ in momentum- and frequency-space, where $\epsilon(q,\omega)$ is the dielectric function and $v_q = 4\pi/q^2$ the bare Coulomb interaction. While there have been many works focusing on higher order (vertex) corrections to the self-energy,[9,10] here we keep only the leading term first order in W, i.e., $\Sigma = iGW$, yielding the GW approximation of Hedin.[11,12]

The GW approximation has been highly successful e.g., for quasi-particle properties such as corrections to DFT calculations of band-gaps, and has also been extended to finite temperatures.[13,14] On the other hand, the GW self-energy $\Sigma(k,\omega)$ is state and frequency dependent, and its calculation is computationally demanding. In an attempt to develop a more efficient approximation, the static COHSEX has been introduced, in which the screened Coulomb interaction $W(q,\omega)$ is replaced by its static limit $W(q,0)$, and the self-energy Σ is split into statically screened exchange (SEX) and Coulomb-hole (COH) terms.[12] Although the separation into exchange and correlation parts is arbitrary, depending on the treatment of exchange, the explicit separation of the COH and SEX contributions in the COHSEX approximation is physically motivated,[12,15] and serves to elucidate the nature of exchange and correlation effects in the theory.

Since its inception, the $T = 0$ COHSEX approximation has been well studied.[12,16] however, its behavior at finite-temperature has heretofore been unexplored. The main goal of this paper is therefore to develop the FT generalization of the COHSEX approximation, and to assess it's accuracy. Our approach is based on an extension of the FT GW approximation to the self-energy.[17] We present a systematic analysis similar to that for $T = 0$, comparing the static COH and SEX approximations with the fully dynamic GW quasiparticle self energy. We also present a brief analysis of the physical basis of these results. As in other investigations of the GW approximation,[7,10,13] we limit our explicit calculations here to the homogeneous electron gas (HEG). However, the approach can be applied more generally as an approximation to the GW self-energy.

The remainder of the paper is organized as follows: in the next section we review the $T = 0$ case and present the FT generalizations of the GW and static COHSEX approximations. Subsequent sections discuss the static and fully dynamic results, followed by an analysis and a summary and conclusions. Throughout this paper we use Hartree atomic units $e = \hbar = m = 1$, with energies in Hartrees and distances in Bohr, unless otherwise noted.

II. COHSEX APPROXIMATION

A. Zero-temperature

We begin with a summary of results for the GW self energy and the COHSEX approximation at $T = 0$. All the quantities discussed in this limit are time-ordered, as in standard zero-temperature many-body perturbation theory. Formally, the GW approximation to the quasiparticle self-energy in momentum-k and frequency-ω space at $T = 0$ is the GW self-energy given by[11,12]

$$\Sigma^T(k,\omega) = \int \frac{d^3q\ d\omega'}{(2\pi)^4}\, G_0^T(\mathbf{k}-\mathbf{q},\omega-\omega')\times \\ \times W^T(q,\omega')e^{-i\omega'\delta^+}, \qquad (1)$$

where G_0^T is the non-interacting, time-ordered one-particle Green's function and W^T the time-ordered, dynamically screened Coulomb interaction. For a given dielectric function $\epsilon(q,\omega)$, the screened interaction W^T can be expressed in terms of its spectral representation

$$W^T(q,\omega) = v_q + W_p^T(q,\omega), \tag{2}$$

$$W_p^T(q,\omega) = \int_{-\infty}^{\infty} d\omega' \frac{D(q,\omega')}{\omega-\omega'+i\delta\,\mathrm{sgn}(\omega')}, \tag{3}$$

where $D(q,\omega) = (1/\pi)|\mathrm{Im}\,W^T(q,\omega)|\,\mathrm{sgn}(\omega)$ is the anti-symmetric (in frequency) bosonic excitation spectrum and $W_p^T(q,\omega)$ the polarization part of W^T. Thus the poles of $W^T(q,\omega)$ in the ω-plane correspond to the peaks in the loss function $(1/\pi)\left|\mathrm{Im}\,\epsilon^{-1}(q,\omega)\right|$. Formally the GW self-energy Σ can be partitioned into fully dynamic screened exchange (SEX) and Coulomb-hole (COH) terms, which are defined from the poles of G_0^T and those of W^T respectively.[11] At zero temperature this yields the exact separation $\Sigma^T(k,\omega) = \Sigma^{SEX,T}(k,\omega) + \Sigma^{COH,T}(k,\omega)$ where

$$\Sigma^{SEX,T}(k,\omega) = -\int \frac{d^3q}{(2\pi)^3} f(\varepsilon_{\mathbf{k-q}}) W^T(q,\omega-\varepsilon_{\mathbf{k-q}}), \tag{4}$$

$$\Sigma^{COH,T}(k,\omega) = \int \frac{d^3q}{(2\pi)^3}\int_0^{\infty} d\omega' \frac{D(q,\omega')}{\omega-\varepsilon_{\mathbf{k-q}}-\omega'+i\delta}. \tag{5}$$

The COHSEX approximation to the quasi-particle self-energy, is then defined as the statically screened approximation to the on-shell GW self-energy $\Sigma(k,E_k)$, where the quasi-particle energy satisfies $E_k = \varepsilon_k + \Sigma(k,E_k)$. The bosonic spectral function $D(q,\omega)$ becomes small at large q; if this decay is sufficiently rapid, then since $E_k \approx k^2/2$ one can to a good approximation replace $\omega - \varepsilon_{\mathbf{k-q}} \approx 0$ in W in Eq. (4) and (5).[12] Then, using the spectral representation of W, the static COH and SEX approximations, which are independent of frequency ω, can be denoted with a subscript k and given by

$$\Sigma_k^{SEX} = -\int \frac{d^3q}{(2\pi)^3} f(\varepsilon_{\mathbf{k-q}}) W^T(q,0), \tag{6}$$

$$\Sigma_k^{COH} = \frac{1}{2}\int \frac{d^3q}{(2\pi)^3} W_p^T(q,0), \tag{7}$$

where $f(\varepsilon) = \theta(\mu-\varepsilon)$ is the zero-temperature Fermi factor. The factor $1/2$ is due to the anti-symmetry of $D(\omega)$ about $\omega = 0$, and has been attributed to the adiabatic turn on of the screened interaction.[12] Their sum is referred to as the static COHSEX self-energy

$$\Sigma_k^{COHSEX,T} \equiv \Sigma_k^{COH,T} + \Sigma_k^{SEX,T}. \tag{8}$$

This approximation is often used as an efficient method for obtaining quasiparticle corrections $\Delta_k = E_k - \varepsilon_k$ to DFT single-particle energies ε_k, since it obviates the necessity of calculating dynamic screening. Indeed, the calculation of the dynamically screened Coulomb interaction W is by far the most computationally demanding part of GW calculations, where typically of $O(10^2)$ frequency points are required for converged results for the fully dynamic quasi-particle self energy with $\omega = E_k$ from Eq. (4) and (5).[12] Thus the static approximation can reduce the computational cost immensely. Nevertheless the static COHSEX approximation turns out to be fairly rough, and cannot be relied on, e.g. for accurate calculations of band gaps, as discussed below. Recently, Kang and Hybertsen,[16] have investigated the errors in the static COHSEX approximation at $T = 0$ by comparing each contribution to the corresponding term in the full GW quasiparticle energy. They found that while the static SEX approximation is generally a good approximation to the fully dynamic SEX, the static Coulomb hole approximation yields errors of order 10-20% to the fully dynamic COH terms for the occupied states. In addition, they suggest a method for correcting the static COH term which give significant improvements for both occupied and low lying unoccupied states.

B. Finite-temperature

We now derive the finite temperature generalization of the static COHSEX approximation to the GW quasi-particle self-energy. Our treatment follows *mutatis, mutandis*, from the zero-temperature theory with FT generalizations of G_0^T, W^T and Σ^T. Additional details are given in the Appendix. To this end, we replace the time-ordered quantities in Eq. (1) with Matsubara quantities,[18]

$$\Sigma^M(k,i\omega) = -k_BT\int \frac{d^3q}{(2\pi)^3}\sum_{n_{even}} G_0^M(k+q,i\omega+i\omega_n) \times W^M(q,i\omega_n). \tag{9}$$

Then taking the analytic continuation to the real-ω axis, the fully dynamic FT retarded self-energy Σ^R in the GW approximation is given by[19]

$$\Sigma^R(k,\omega,T) = \int_0^{\infty} d\omega' \int \frac{d^3q}{(2\pi)^3} D(q,\omega') \times \times\left[\frac{f(\epsilon_{\mathbf{k-q}})+N(\omega')}{\omega+\omega'-\epsilon_{\mathbf{k-q}}+i\delta} + \frac{1-f(\epsilon_{\mathbf{k-q}})+N(\omega')}{\omega-\omega'-\epsilon_{\mathbf{k-q}}+i\delta}\right], \tag{10}$$

where $f(\varepsilon) = 1/[e^{\beta(\varepsilon-\mu)}+1]$ is the Fermi factor, $\mu = \mu(T)$ the chemical potential, and $N(\omega) = 1/[e^{\beta\omega}-1]$ the Bose factor, each with implicit temperature and electron density dependence, $\beta = 1/k_BT$ and $n = N/V = 3/4\pi r_s^3$ in the thermodynamic limit. The static exchange term is given by $\Sigma^x(k,T) = \int [d^3q/(2\pi)^3] f(\epsilon_{\mathbf{k-q}}) v_q$. The spectral function D has implicit temperature dependence from that of the RPA dielectric function $\epsilon(q,\omega,T)$,

$$\epsilon(q,\omega,T) = 1 + 2v_q\int \frac{d^3k}{(2\pi)^3}\frac{f(\varepsilon_{k+q})-f(\varepsilon_k)}{\omega-\varepsilon_{k+q}+\varepsilon_k}, \tag{11}$$

The imaginary part of $\epsilon(q,\omega,T)$ is analytic,[20,21] and the real part is calculated via a Kramers-Kronig transform.

As in the $T = 0$ case, the fully dynamic self-energy at finite temperature and it's COH and SEX parts are obtained by evaluating the poles of G_0 and W respectively. The SEX terms with the Fermi factor arise from G_0, while the COH terms with the Bose factors come from the screened Coulomb interaction W. Separating these contributions in the fully dynamic FT quasi-particle GW retarded self-energy yields

$$\Sigma^{SEX,R}(k,\omega) = -\int \frac{d^3q}{(2\pi)^3} f(\varepsilon_{\mathbf{k-q}}) W^R(q,\omega-\varepsilon_{\mathbf{k-q}}) \quad (12)$$

$$\Sigma^{COH,R}(k,\omega) = \int_0^\infty d\omega' \int \frac{d^3q}{(2\pi)^3} D(q,\omega') \times \times \left[\frac{N(\omega')}{\omega+\omega'-\varepsilon_{\mathbf{k-q}}+i\delta} + \frac{1+N(\omega')}{\omega-\omega'-\varepsilon_{\mathbf{k-q}}+i\delta} \right]. \quad (13)$$

At finite T, Eq. (12) is identical in form to Eq. (4), apart from implicit temperature dependence in $f(\varepsilon)$ and $W^M(q,\omega)$. Eq. (13) reduces to Eq. (5) at $T = 0$; however, the Bose factors $N(\omega)$ become increasingly important at finite T. In the limit of static screening, we therefore obtain the FT generalization of the COHSEX approximation. The real parts of the FT COHSEX approximation to Σ_k are similar to those for $T = 0$ in Eq. (6) and (7)

$$\Sigma_k^{SEX}(T) = -\int \frac{d^3q}{(2\pi)^3} f(\varepsilon_{\mathbf{k-q}}) W^R(q,0), \quad (14)$$

$$\mathrm{Re}\left[\Sigma_k^{COH}(T)\right] = \frac{1}{2}\int \frac{d^3q}{(2\pi)^3} W_p^R(q,0). \quad (15)$$

As at $T = 0$ the static exchange term is given by $\Sigma^x(k,T) = \int [d^3q/(2\pi)^3] f(\varepsilon_{\mathbf{k-q}}) v_q$. However, in contrast to the zero temperature case, the static approximation for the FT COH term is complex valued, with a negative imaginary part given by

$$\mathrm{Im}\left[\Sigma_k^{COH,R}(T)\right] = -\int \frac{d^3q}{(2\pi)^2} \lim_{\omega\to 0^+} N(\omega) D(q,\omega). \quad (16)$$

Note that at low frequency, $D_q(\omega) \propto \omega$ due to particle-hole continuum excitations and $N(\omega) \to k_BT/\omega$ mirrors the high temperature behavior. Thus, the imaginary part of the static COH contribution to Σ increases with temperature. Explicit calculations, however, show that the imaginary part of the static COH term is quite small at all temperatures compared to the contribution from the dynamic COHSEX term.

III. STATIC VS DYNAMIC COHSEX

As an illustration of the FT theory, we first compare the static and fully dynamic SEX and COH contribution to the quasi-particle GW self-energy on the energy shell $\Sigma_k = \Sigma(k, E_k)$ for the homogeneous electron gas (Fig. 1 top) from Eq. (11-14). For all cases the agreement between static and fully dynamic SEX contribution is quite good, both at low and high k, and become increasingly accurate with increasing temperature. On the other hand the COH terms dominate the GW self-energy Σ_k for all k, but there are substantial errors in making the static approximation at low temperatures, which become smaller with increasing temperature. The dispersion of the fully dynamic COH and SEX contributions largely cancels for $k < k_F$ at low temperature. However, this cancelation does not persist at higher temperatures ($T/T_F > 0.5$), where the dispersion of both contributions is positive. It is important to note that the static COH contribution Σ_k^{COH} is actually constant, independent of k, and hence entirely local. In contrast the dynamic COH terms become strongly momentum dependent beyond a cross-over point $k_p = [2(\omega_p + \varepsilon_F)]^{1/2}$, corresponding to the onset of plasmon-excitations, with the real part approaching zero asymptotically at high momenta and the imaginary part becoming large. Thus for unoccupied states at high $k > k_p$ dynamic corrections to the COHSEX approxima-

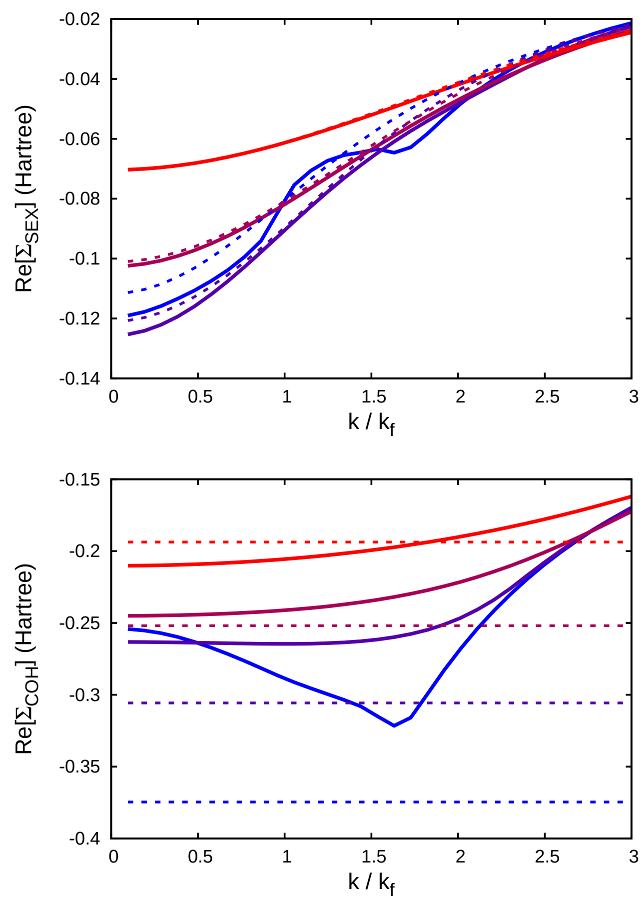

FIG. 1. (Color online) Results for the SEX (top) and COH (bottom) contributions to the static (dashed) and full dynamic (solid) quasiparticle self-energy vs k/k_F at various temperatures T/T_F for the homogeneous electron gas for $r_s = 2.0$: (from blue to red) the curves denote T/T_F =0.01, 0.5, 1.0, and 2.0. Note that the COH contribution is always significantly larger in magnitude than the SEX and persists to higher k/k_F, while the SEX becomes for unoccupied states above k_F.

tion are essential, and necessary to account for the substantial broadening of the high energy unoccupied states.

This behavior is illustrated in Fig. 2 with a comparison between the static total static COHSEX and and fully dynamic self-energy for various densities $r_s = 1, 2, 3$ and 4, and $T/T_F = 0.01$ and 1. Note also that the static approximation exhibits considerably less variation with respect to r_s, k, and T than the fully dynamic results. At high T, the dispersion in the quasi-particle self-energy Σ_k is also fairly well represented by the total static COHSEX for $k < k_p$, and has a much smoother variation with temperature than the low T behavior. For comparison we also show the FT-DFT exchange-correlation potential v_{xc} for $r_s = 4$. As expected, the value of v_{xc} is nearly identical to the quasiparticle energy correction at the $k = k_F$. However, at high T, the Fermi surface broadens and ceases to be a precisely defined concept, and the chemical potential can even lie below the bottom of the band. Thus at high T, $v_{xc}(T)$ is no longer equivalent to the quasiparticle correction at the Fermi level. Although the static COHSEX approximation captures much of the quasi-particle correction to the DFT, significant errors remain, especially for excited states at high $k > k_p$. We show in Fig. 3 the imaginary part of the quasi-particle self-energy $|\mathrm{Im}\,\Delta_k = \mathrm{Im}\,\Sigma_k|$ vs temperature from the COH (solid) and SEX (dashed) contributions at various temperatures. Unlike the fully dynamic results, the static COHSEX has zero imaginary part at $T = 0$, while at finite T, the COH term alone contributes, resulting in a value of $\approx -0.02i$ H at $T/T_F = 4$, i.e., about 10% of the GW self-energy.

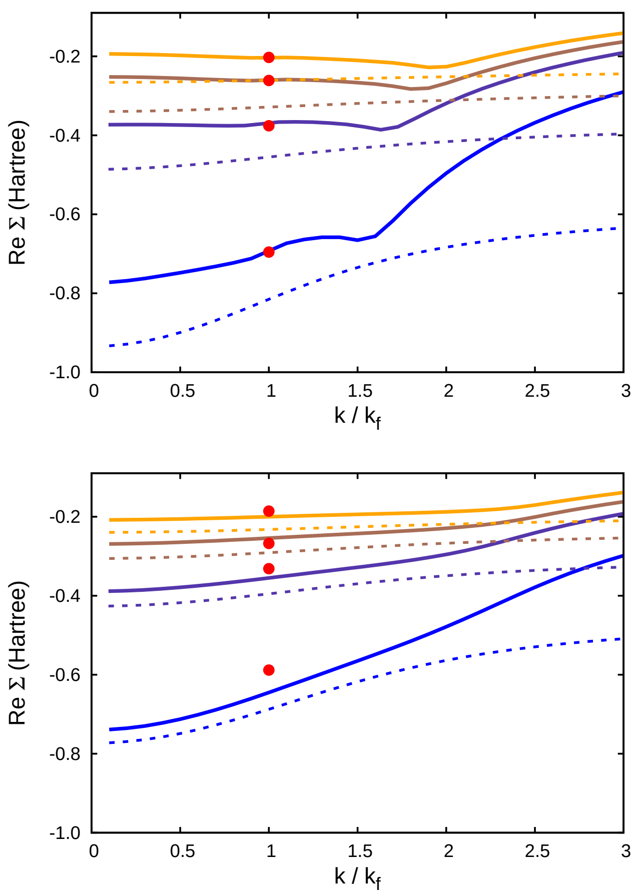

FIG. 2. (Color online) The real part of static COHSEX approximation (dashed) vs fully dynamic self-energy (solid) for various densities: (from blue to orange) r_s =1.0, 2.0, 3.0, 4.0 at $T/T_F = 0.01$ (top) and 1.0 (bottom). Note that the high temperature behavior is considerably smoother than near $T = 0$ and the change in behavior beyond about $k = k_p$ reflecting the onset of plasmon excitations. For reference the LDA-$v_{xc}(T)$[5,17] for each r_s are added as circles at k_F.

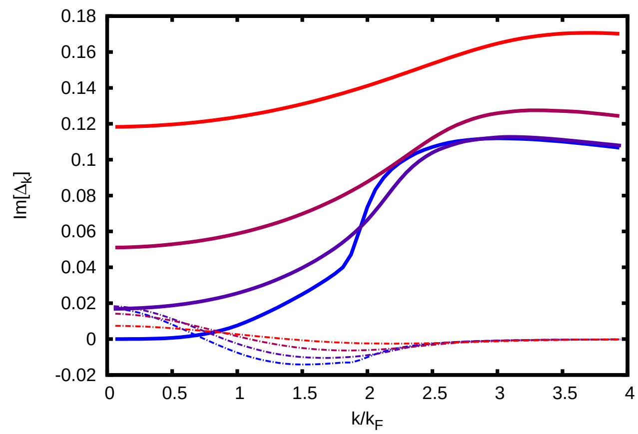

FIG. 3. (Color online) Fully dynamic COH (solid) and SEX (dashed) contributions to the imaginary part of the quasiparticle correction to the DFT energy ε_k vs k/k_F for $r_s = 4.0$, for various temperatures: (from blue to red) T/T_F =0.01, 0.5, 1.0, and 2.0. Note that the dominant contribution comes from the COH terms, while the dynamic contributions to the SEX from particle-hole excitations are significant only near k_F

IV. ANALYSIS

In an effort to better understand the static COHSEX approximation and dynamic corrections to the GW self energy, we now present a brief analysis. Physically the GW approximation describes the quasi-particle self-energy due to a dynamically screened exchange-correlation hole. The separation into COH and SEX terms arises naturally in the GW approximation from the poles of W and those of G_0 respectively. The static approximations then amount to replacing the frequency argument of $W(q, E_k - \varepsilon_{\mathbf{k-q}})$ with zero. Thus the static FT screened Coulomb interaction $W(q, 0) = 4\pi/[q^2 + \kappa(T)^2]$ has a temperature dependent screening constant $\kappa(T)$ that varies from the Thomas-Fermi value at $T = 0$ to the Debye-Hückel limit at high T.[3,17] The FT behavior of the loss function $L(q, \omega) = |\mathrm{Im}\,\epsilon^{-1}(q, \omega)|$ is illustrated in Fig. 4. At high temperature, higher energy plasmons contribute less to the full COH due to the broadening.

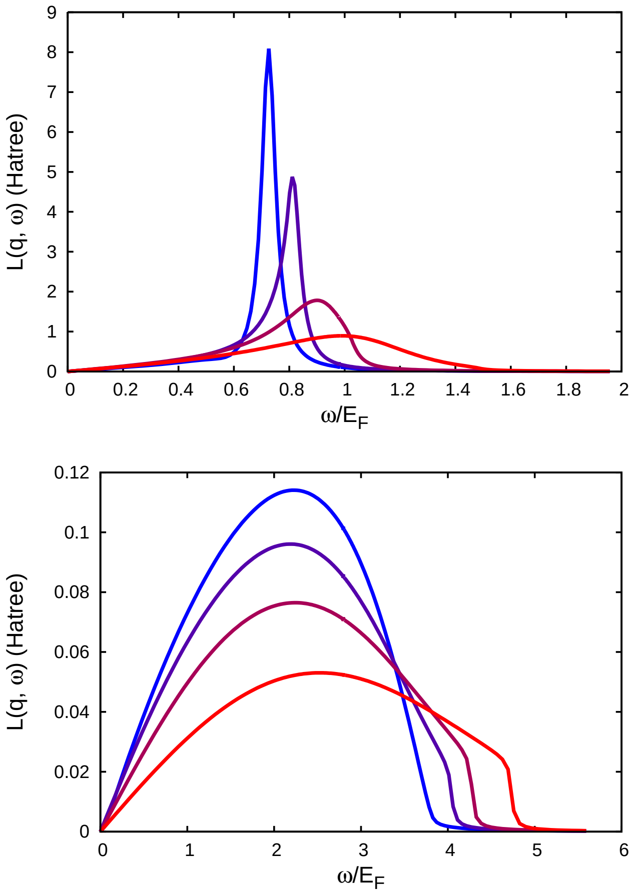

FIG. 4. (Color online) The electron energy-loss function $L(q,\omega) = |\mathrm{Im}\ \epsilon^{-1}(q,\omega)|$ for $r_s = 2.0$ at various temperatures: (from blue to red) T/T_F =0.01, 0.5, 1.0, and 2.0 for momentum $q/k_F = 0.5$ (top) and 2.0 (bottom).

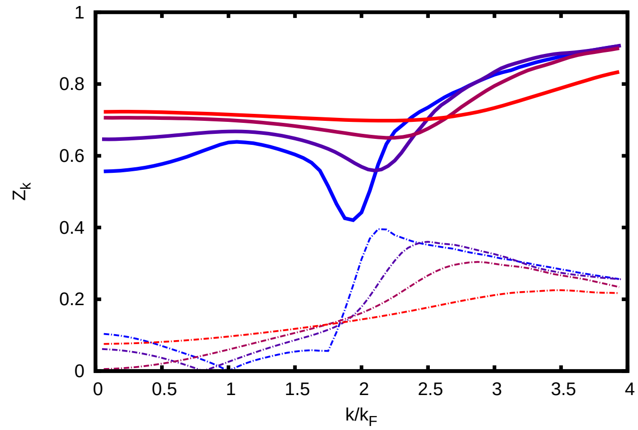

FIG. 5. Real (solid) and imaginary (dashed) parts of the renormalization constant Z_k vs k/k_F for r_s=4.0 at (blue to red) T/T_F =0.01, 0.5, 1.0, and 2.0.

By examining Eq. (15), the full COH gets closer to the static COH as the blue-shifted plasmons contributes less to adiabatic accumulation of the Coulomb hole from W_p.

Why is the static approximation so good for the SEX term, while at best only fair for the COH term and only for the occupied levels? In an attempt to answer this question, we examine Eq. (12) and (13) in the limit of zero momentum and low temperature, as investigated in detail e.g., by Lundqvist.[22] for the $T = 0$ case. For the SEX term, the Fermi function and the screened Coulomb potential have the same argument $q^2/2$, up to a sign. As a result, the frequency argument in $W(q,\omega)$ is limited to $\omega < \epsilon_F$, and hence the substantial variation of W near the plasmon excitation energy ω_p - which is usually larger than the Fermi energy ϵ_F for low to normal ($r_s \approx 2-6$) densities - is never accessed. At high momenta $k/k_F \gg 1$, the Fermi function acts to ensure that q/k_F must also be large for any significant contribution. Consequently the frequency argument of W is large only when the momentum is also large. This suppresses the matrix element in the total since $W(q,\omega) \propto 1/q^2$ for large q. Consequently dynamic corrections are small for the SEX term. In contrast, the static COH term in Eq. (13) has no limitations on the arguments of $W(q,\omega)$. Physically, the dynamic contributions to the SEX arise only from low energy excitations, e.g., the particle-hole continuum. In contrast the dynamic COH term includes excitations at all energies and its dynamic contributions are dominated by plasmon-excitations and to a much lesser extent particle-hole excitations. These effects are evident in the imaginary part of the self-energy (Fig. 3), where $\mathrm{Im}\,\Sigma^{SEX}(k,E_k)$ is limited to momenta near or below k_F, while that for $\Sigma^{COH}(k,E_k)$ is appreciable even beyond the onset of plasmon excitations k_p. Another consequence of the static approximation is that the COH contribution is completely local, i.e., k-independent. This is a drastic approximation, and fails to account for the substantial variation of the self-energy for $k > k_p$ due to plasmon excitations.

Although the COHSEX approximation is perhaps most useful for estimates of the quasi-particle self energy, it is interesting to consider other corrections to the quasi-particle approximation at finite T. These are reflected for example, in the the renormalization factor $Z_k = [1 - \partial\Sigma(k,\omega)/\partial\omega]^{-1}_{\omega=\varepsilon_k}$. Since deviations of Z_k from unity correspond to the fraction of satellites in the spectral function, Z_k provides a diagnostic of the validity of the quasiparticle approximation. For a more detailed analysis and illustrations of the behavior of the finite-T spectral function, we refer the reader to Ref17 and 23. Fig. (5) shows the renormalization factor as a function of k for $r_s = 4.0$ and T/T_F =0.01, 0.5, 1.0, and 2.0. Clearly the quasiparticle approximation becomes increasingly valid for very high energy states well above the plasmon frequency $\varepsilon_k \gg \omega_p$. However, this is the range for which the static COH has the largest errors. Since deviations of Z_k from unity correspond to the fraction of satellites in the spectral function, Z_k provides a diagnostic of the validity of the quasiparticle approximation. For a more detailed analysis and illustrations of the behavior of the

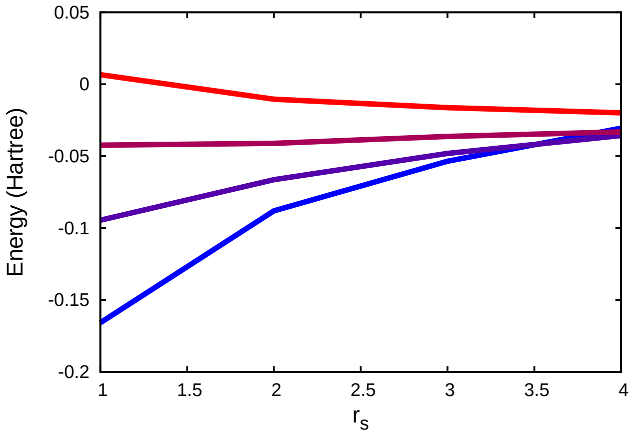

FIG. 6. (Color online) Dynamic correction to COHSEX self-energy $\Sigma(k, E_k) - \Sigma_k^{COHSEX}$ at the Fermi level k_F as a function of r_s: from blue to red, the curves denote T/T_F =0.01, 0.5, 1.0, and 2.0.

finite-T spectral function, we refer the reader to Refs. 17 and 23. Note in addition that the renormalization constant is $Z_k \approx 0.75$ for $r_s = 4$, even at high T/T_F, indicating that the quasiparticle energy correction is reduced in magnitude compared to that calculated at the bare energy. This suggests that errors in the static COHSEX approximation of order 20% may well be a best case scenario. Thus while the renormalization constant shows the importance of satellites in the single particle spectrum, it is not a good diagnostic for the quality of the static approximation to the quasiparticle energies.

Finally, Fig. 6 shows the magnitude of the dynamic corrections to the static COHSEX self-energy at the Fermi momentum as a function of r_s. These results show that for all temperatures, the dynamic correction is smoothly decreasing (increasing) with increasing r_s for $T > (<) T_F$. This behavior suggests that a simple additive correction to the DFT exchange correlation potential may be a reasonable approximation to correct the static COHSEX approximation for states $0 < k < k_p$.

V. SUMMARY AND CONCLUSIONS

We have generalized the COHSEX approximation to the GW self-energy to finite temperatures, with an explicit treatment of both the COH and SEX contributions. We find that the FT COHSEX approximation is similar in many-respects to that for $T = 0$. Formally the separation of the fully dynamic GW self-energy into COH and SEX terms and their definitions are similar to their counterparts at $T = 0$, apart from explicit temperature dependence in their ingredients. The static SEX approximation continues to be a very good approximation to the fully dynamic SEX over a broad range of densities, temperatures, and momenta, but is only substantial for occupied levels below about k_F. The COH term is generally much larger than the SEX and persists to higher energies, with a cross-over at the onset of plasmon excitations at $k = k_p$. While the static COH approximation is only fair for mostly occupied and low-lying unoccupied states $k < k_p$ at low temperture, it completely fails to describe dynamic effects in the $\Sigma^{COH}(k, E_k)$ at high $k > k_p$. This behavior is similar to that in the analysis by Kang and Hybertsen for the $T = 0$ case.[16] However, a key difference for finite-T is that the static COHSEX approximation becomes complex valued, even at the Fermi level, with an imaginary part that grows with temperature. While these deficiencies can be remedied for the nominally occupied states, e.g., by generalizing the extended COHSEX approximation[16] to finite temperature, the static COH approximation still retains it's unphysical spatial locality, independent of k. This limitation has the consequence that at high T, equilibrium properties will be increasingly error-prone since they depend on the high momentum behavior of the electrons. Nevertheless, the static COHSEX approximation does provide a fair approximation of corrections to DFT for quasi-particle energies with typical errors of about 10-20%. While this degree of accuracy provides rough estimates of quasi-particle corrections to DFT, dynamic corrections are always important.

Acknowledgments: We thank M. Hybertsen and L. Reining for comments. This work is supported by the DOE Office of Science BES Grant DE-FG02-97ER45623.

Appendix A: Derivation of static COHSEX approximation

In this section, we present some additional details of the derivation of the static FT COHSEX approximation from the fully dynamic FT quasi-particle COHSEX self-energy. Starting from Eq. (12) and (13) and using the Sokhotski-Plemelj formula, we can separate the COH term into real and imaginary parts as

$$\mathrm{Re}[\Sigma^{COH}(k,\omega)] = \mathcal{P}\int_0^\infty d\omega' \int \frac{d^3q}{(2\pi)^3} D(q,\omega') \times \\ \times \left[\frac{N(\omega')}{\omega+\omega'-\varepsilon_{\mathbf{k-q}}} + \frac{1+N(\omega')}{\omega-\omega'-\varepsilon_{\mathbf{k-q}}}\right] \quad \text{(A1)}$$

$$\mathrm{Im}[\Sigma^{COH}(k,\omega)] = -\pi\int_0^\infty d\omega' \int \frac{d^3q}{(2\pi)^3} D(q,\omega') \times \\ \times \Big[N(\omega')\delta(\omega+\omega'-\varepsilon_{\mathbf{k-q}}) + \\ + [1+N(\omega')]\,\delta(\omega-\omega'-\varepsilon_{\mathbf{k-q}})\Big], \quad \text{(A2)}$$

where $\mathcal{P}$ denotes the principal value. To further simplify Eq. (A2), we use the anti-symmetric property of $D(q,\omega)$

and $N(-\omega) = -1 - N(\omega)$, so that

$$\begin{aligned}\mathrm{Im}[\Sigma^{COH}(k,\omega)] = &-\pi\int\frac{d^3q}{(2\pi)^3}\Big[D(q,\varepsilon_{\mathbf{k-q}}-\omega)\times \\ &N(\varepsilon_{\mathbf{k-q}}-\omega)\theta(\varepsilon_{\mathbf{k-q}}-\omega)+ \\ &D(q,\omega-\varepsilon_{\mathbf{k-q}})\times\big[1+N(\omega-\varepsilon_{\mathbf{k-q}})\big]\theta(\omega-\varepsilon_{\mathbf{k-q}})\Big] \\ = &-\pi\int\frac{d^3q}{(2\pi)^3}\big[D(q,\varepsilon_{\mathbf{k-q}}-\omega)N(\varepsilon_{\mathbf{k-q}}-\omega)\big]. \quad \text{(A3)}\end{aligned}$$

In the limit of static screening ($\omega - \varepsilon \to 0^+$), the imaginary part is found by evaluating $D(q,\omega)$ and $N(\omega)$ at low frequency: $D(q,\omega) \propto \omega$ due to particle-hole continuum excitations, and $N(\omega) \to k_BT/\omega$ because k_BT is large compared to $\omega \to 0^+$ for $T > 0$. On the other hand, the Bose factors in the real part cancel identically for all ω' after taking the static limit, so we end up with the same form as in the zero temperature limit, up to the temperature dependence of the screened coulomb interaction. Therefore, the FT static COHSEX becomes

$$\mathrm{Re}[\Sigma^{SEX}(k)] = -\int\frac{d^3q}{(2\pi)^3}f(\varepsilon_{\mathbf{k-q}})\mathrm{Re}[W_M(q,0)], \quad \text{(A4)}$$

$$\begin{aligned}\mathrm{Re}[\Sigma^{COH}(k)] &= \mathcal{P}\int_0^\infty d\omega'\int\frac{d^3q}{(2\pi)^3}D(q,\omega')\times \\ &\times\left[\frac{N(\omega')}{\omega'}+\frac{1+N(\omega')}{-\omega'}\right] \\ &= \mathcal{P}\int_0^\infty d\omega'\int\frac{d^3q}{(2\pi)^3}\frac{D(q,\omega')}{-\omega'} \\ &= \frac{1}{2}\int\frac{d^3q}{(2\pi)^3}W_p(q,0). \quad \text{(A5)}\end{aligned}$$

$$\mathrm{Im}[\Sigma^{SEX}(k)] = -\int\frac{d^3q}{(2\pi)^3}f(\varepsilon_{\mathbf{k-q}})\mathrm{Im}[W(q,0)] = 0, \quad \text{(A6)}$$

$$\begin{aligned}\mathrm{Im}[\Sigma^{COH}(k)] &= -\pi\int\frac{d^3q}{(2\pi)^3}\lim_{\omega'\to0^+}D(q,\omega')N(\omega') \\ &= -\pi k_BT\int\frac{d^3q}{(2\pi)^3}\alpha(\mathbf{q}), \quad \text{(A7)}\end{aligned}$$

where $\alpha(q) = dD(q,\omega)/d\omega|_{\omega=0}$ is the proportionality constant. While the imaginary part of the static COH is linear in temperature, it is relatively small compared to the fully dynamic FT quasi-particle self-energy. To complete the derivation, we then use the following relations to convert the retarded static COHSEX results into time-ordered quantities

$$\mathrm{Re}[G_R(k,\omega)] = \mathrm{Re}[G_T(k,\omega)], \quad \text{(A8)}$$

$$\mathrm{Im}[G_R(k,\omega)] = \coth(\omega/2T)\ \mathrm{Im}[G_T(k,\omega)]. \quad \text{(A9)}$$

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