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Temperature dependence of the Hartree-Fock approximation

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The Hartree-Fock exchange energy of the electron gas is calculated at nonzero temperatures. The calculation is done self-consistently in that the Hartree-Fock self-energy is included self-consistently in the Fermi-Dirac occupation numbers. We also calculate the first and second derivatives of the Hartree-Fock exchange energy with respect to density, which are useful for density-functional calculations at nonzero temperatures.

I. INTRODUCTION

The homogeneous electron gas[1] is the standard model in which to investigate electron-electron interactions. The positive charges are spread uniformly throughout the sample and the difficult problems are due to electron-electron interactions. The lowest level of approximation is to include only electron exchange, which is called the Hartree-Fock approximation (HFA). In the approximation, the Hartree-Fock exchange energy is given by

$$E_g = -\frac{1}{\nu}\sum_{\mathbf{pq}} v_{\mathbf{q}} n_{\mathbf{p}} n_{\mathbf{p+q}}, \tag{1}$$

where $v_{\mathbf{q}} = 4\pi e^2/q^2$ in three dimensions and ν is the volume. At zero temperature, the Fermi-Dirac occupation functions are $n_{\mathbf{p}} = \theta(k_F - p)$, a step function at the Fermi wave vector k_F. Here we wish to consider the evaluation of the Hartree-Fock exchange energy at nonzero temperatures.

Most previous evaluations[2–10] of this expression at nonzero temperatures have just used the noninteracting occupation function ($n_{\mathbf{p}} = 1/\{\exp[\beta(\varepsilon_{\mathbf{p}} - \mu)] + 1\}$), where μ is the chemical potential, $\varepsilon_{\mathbf{p}} = \hbar^2 p^2/2m$, and $\beta = 1/k_B T$. This procedure is the correct result in the first order of perturbation theory. Here we wish to include more terms in perturbation theory. As a way to include higher-order terms effectively, Lidiard[11] suggested a good variational form of the Fermi-Dirac function, where β was considered to be a variational parameter, which was followed by Umeda and Tomishima.[12]

Since exchange effects change the particle energy and the occupation number corresponding to it, we do the calculation self-consistently by including the Hartree-Fock self-energy $\Sigma_x(p)$ in the argument of the occupation numbers. In order to count correctly, the higher-order diagrams, we must include the self-energy while performing a coupling constant integral.[13–15] Much earlier work by Wohlfarth,[16] Lidiard,[17] and Cowan and Ashkin[18] also included the self-energy self-consistently. The approach by Lidiard[17] was analytical, and limited to various cases of very high and very low temperatures. We use the computer to evaluate these expressions for a full range of temperatures.

There are two different applications of self-energies at nonzero temperatures. One is astrophysical, where one models stars and other galactic phenomena. The second is in condensed matter physics. Many calculations are done using the local density approximation (LDA) of Hohenberg, Kohn, and Sham.[19] For a recent review, see Mahan and Subbaswamy.[20] The Hartree-Fock exchange energy plays an important role in LDA calculations. The LDA formalism for nonzero temperatures was formally set up by Mermin.[21] There is some interest in doing LDA at nonzero temperatures, in which case one needs the Hartree-Fock exchange energy at nonzero temperatures. This latter application is of interest here. We also calculate the first and second derivatives of the Hartree-Fock exchange energy with respect to density.

Here we generalize the previous work by Gupta and Rajagopal[8] (to be referred to as GR) who proposed the exchange-only scheme, where they used the exchange energy $E_x(n,T)$ with the noninteracting occupation function $n_{\mathbf{p}}$ as in many previous works. This $E_x(n,T)$ was the same as E_g/ν. But in our calculations we include the Hartree-Fock self-energy $\Sigma_x(p)$ in the argument of the occupation numbers while doing a coupling-constant integration. The correct Fermi-Dirac function, which we call $F(p)$, contains the exchange self-energy $\Sigma_x(p)$ in its argument:

$$F(p) = \frac{1}{e^{\beta E(p)} + 1}, \tag{2}$$

where $E(p) = \varepsilon_{\mathbf{p}} + \Sigma_x(p) - \mu$ is the particle energy.

The aim of this paper is to give a full self-consistency to

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the previous formalism by GR by expressing the Hartree-Fock exchange energy $E_x(n,T)$ as a integral over the coupling constant, with the correct Fermi-Dirac function $F(k)$ including the self-energy in its argument. In Sec. II, the nonzero temperature formalism calculating $E_x(n,T)$ and its derivatives with respect to density is developed. In Sec. III, the paramagnetic susceptibility of an interacting electron gas is obtained and some differences between our results and those of GR are discussed. In the Appendixes, some notes and comments are given for the thermodynamic potential and the Lindhard function.

II. THEORY : TEMPERATURE DEPENDENCE OF HFA

We consider a homogeneous electron gas without external potential. The Hartree potential of the electron gas is canceled by charge neutrality. In this paper, we consider only exchange effects, neglecting correlation processes. Then we can approximate the effective single-particle potential V_{eff} as only exchange part: $V_{\text{eff}} \simeq V_x(n,T) = \delta\Omega_x(n,T)/\delta n$. $\Omega_x(n,T)$ is the Hartree-Fock contribution to the thermodynamic potential of the system due to exchange effects. In general, the thermodynamic potential $\Omega(n,T)$ is obtained by a coupling constant integration.[13–15] See notes on the thermodynamic potential in Appendix A.

To include correctly the lowest order and all higher-order diagrams with electron exchange effects, we use the self-consistent Hartree-Fock approximation in which the Hartree-Fock exchange energy per volume $E_x(n,T) \equiv \Omega_x(n,T)/\nu$ is given by a integral over the coupling constant η:

$$E_x(n,T) = \frac{1}{\beta\nu}\sum_{\mathbf{p},ip_n}\int_0^1 \frac{d\eta}{\eta}\Sigma_x(\eta,p)\mathcal{G}^{(x)}(\eta,p), \tag{3}$$

where $\mathcal{G}^{(x)}$ is the fully dressed Matsubara Green's function with the exchange self-energy Σ_x:

$$\mathcal{G}^{(x)}(\eta,p) = \frac{1}{ip_n - [\varepsilon_{\mathbf{p}} + \Sigma_x(\eta,p) - \mu]}, \tag{4}$$

$$\Sigma_x(\eta,p) = -\frac{1}{\beta\nu}\sum_{\mathbf{k},ik_n}\eta v_{\mathbf{p}-\mathbf{k}}\mathcal{G}^{(x)}(\eta,k). \tag{5}$$

Here we used the four-vector notation $p \equiv (\mathbf{p}, ip_n)$ in writing the argument of the Green's function and the self-energy for notational convenience

Since the exchange self-energy does not depend upon the energy variable ip_n, the frequency summation of the Green's function $\mathcal{G}^{(x)}$ just gives the occupation number $F(\eta,p) = 1/\{\exp[\beta E(\eta,p)]+1\}$. (Note that the notation p now represents the magnitude of a vector $\mathbf{p}$.) Then

$$\begin{aligned} E_x(n,T) &= \frac{1}{\nu}\sum_{\mathbf{p}}\int_0^1 \frac{d\eta}{\eta}\Sigma_x(\eta,p)F(\eta,p) \\ &= -\frac{1}{\nu^2}\sum_{\mathbf{pk}}\int_0^1 \frac{d\eta}{\eta}\eta v_{\mathbf{p}-\mathbf{k}}F(\eta,p)F(\eta,k), \end{aligned} \tag{6}$$

$$\begin{aligned} \Sigma_x(\eta,p) &= -\int \frac{d^3k}{(2\pi)^3}\eta v_{\mathbf{p}-\mathbf{k}}F(\eta,k) \\ &= -\frac{\eta e^2 k_F}{\pi p}\int_0^\infty \frac{k\,dk}{e^{G(\eta,k)}+1}\ln\left|\frac{p+k}{p-k}\right|, \end{aligned} \tag{7}$$

$$G(\eta,k) = \beta E(\eta,k) = \beta[\varepsilon_{\mathbf{k}} + \Sigma_x(\eta,k) - \mu], \tag{8}$$

$$\mu = \frac{\hbar^2 k_F^2}{2m} - \frac{\eta e^2 k_F}{\pi} + \delta\mu, \tag{9}$$

$$\mu^0 = \frac{\hbar^2 k_F^2}{2m}. \tag{10}$$

Here μ^0 is the Fermi energy, $-\eta e^2 k_F/\pi$ is zero-temperature shift in the chemical potential due to the exchange self-energy, and $\delta\mu$ is nonzero-temperature deviation in the chemical potential, determined by the number conservation. Note that Eqs. (7) and (8) provide the self-consistent equations for Σ_x, G, and F.

We introduce the reduced inverse temperature ξ (or the reduced temperature t) and the reduced radius α:

$$\xi = \frac{\mu^0}{k_B T} = t^{-1}, \tag{11}$$

$$\alpha = \frac{1}{\pi a_B k_F} = \frac{r_s}{(9\pi^4/4)^{1/3}} = \frac{r_s}{6.029}, \tag{12}$$

where a_B is the Bohr radius and r_s is an effective radius which comes from $n^{-1} = 4\pi(r_s a_B)^3/3$, n being the number density. Thus α (or r_s) is small for a high-density electron gas and large for a low-density one. Scaling all momenta by k_F we obtain

$$G(\eta,y) = \beta E(\eta,y) = G_1(\eta,y) + G_2(\eta,y), \tag{13}$$

$$G_1(\eta,y) = \beta(\varepsilon_{\mathbf{k}} - \mu) = \xi g_1(\eta,y) - a, \tag{14}$$

$$g_1(\eta,y) = y^2 - 1 + 2\eta\alpha, \tag{15}$$

$$a = \xi\delta\mu/\mu^0, \tag{16}$$

$$G_2(\eta,y) = \beta\Sigma_x(\eta,y) = 2\eta\xi\alpha g_2(\eta,y), \tag{17}$$

$$g_2(\eta,y) = -\frac{1}{y}\int_0^\infty \frac{x\,dx}{e^{G(\eta,x)}+1}\ln\left|\frac{y+x}{y-x}\right|. \tag{18}$$

The correction of the chemical potential, $\delta\mu$, is determined by the number conservation: $n = \frac{2}{\nu}\sum_{\mathbf{k}}F(\eta,k)$, i.e.,

$$\int_0^\infty x^2 dx F(\eta,x) = \frac{1}{3}. \tag{19}$$

Note that $g_2(\eta,y)$ does not have any explicit dependence of α except in the exponent $G(\eta,x)$.

Above, we used a correct Fermi-Dirac function $F(\eta,k)$, which is different from the noninteracting Fermi-Dirac function $n_{\mathbf{p}}$. The same problem, which we will solve below, was solved by GR just by using the noninteracting Fermi-Dirac function which lacks a full self-consistency. In this paper, we consider the correct Fermi-Dirac function to give a full self-consistency to HFA and see how much difference there is between the two cases.

For $E_x(n,T)$ we obtain

$$E_x(n,T) = E_x(n,0)I(\xi), \tag{20}$$

$$I(\xi) = -2\int_0^1 d\eta \int_0^\infty dy\, y^2 g_2(\eta,y)F(\eta,y), \tag{21}$$

$$E_x(n,0) = -e^2k_F^4/4\pi^3, \tag{22}$$

$$\widehat{E}_x(n,t) = \frac{E_x(n,T)}{E_x(n,0)} = I(\xi). \tag{23}$$

We define the exchange potential $V_x(n,T)$ and the "interaction function" $K_x(n,T)$, which appears in the calculation of response functions.[22] Since we consider $E_x(n,T)$ instead of $\Omega_x(n,T)$, the functional derivatives of Ω_x are replaced by usual derivatives of E_x in the homogeneous limit. Thus we obtain

$$V_x(n,T) = \frac{dE_x(n,T)}{dn} = V_x(n,0)\widehat{V}_x(n,t), \tag{24}$$

$$\widehat{V}_x(n,t) = I(\xi) + \frac{\xi}{2}\frac{dI(\xi)}{d\xi}, \tag{25}$$

$$V_x(n,0) = -(e^2/\pi)(3\pi^2 n)^{1/3}, \tag{26}$$

$$K_x(n,T) = \frac{d^2E_x(n,T)}{dn^2} = K_x(n,0)\widehat{K}_x(n,t), \tag{27}$$

$$\widehat{K}_x(n,t) = I(\xi) + \frac{7\xi}{2}\frac{dI(\xi)}{d\xi} + \xi^2\frac{d^2I(\xi)}{d\xi^2}, \tag{28}$$

$$K_x(n,0) = -(e^2/3\pi)(3\pi^2)^{1/3}n^{-2/3}, \tag{29}$$

where, using a shorthand notation $\partial_\xi = \frac{d}{d\xi}$,

$$\begin{aligned}\partial_\xi I(\xi) = -2\int_0^1 d\eta \int_0^\infty & dy\, y^2[F(\eta,y)\partial_\xi g_2(\eta,y) \\ & + g_2(\eta,y)\partial_\xi F(\eta,y)],\end{aligned} \tag{30}$$

$$\begin{aligned}\partial_\xi^2 I(\xi) = -2\int_0^1 d\eta \int_0^\infty & dy\, y^2[F(\eta,y)\partial_\xi^2 g_2(\eta,y) \\ & + 2\partial_\xi g_2(\eta,y)\partial_\xi F(\eta,y) + g_2(\eta,y)\partial_\xi^2 F(\eta,y)].\end{aligned} \tag{31}$$

Note that α has ξ dependence through k_F: $\partial_\xi\alpha = -\alpha/2\xi$. The following equations determine $\partial_\xi G(\eta,y)$ and $\partial_\xi^2 G(\eta,y)$:

$$\begin{aligned}\partial_\xi G(\eta,y) = {} & g_1(\eta,y) - \eta\alpha + \eta\alpha g_2(\eta,y) \\ & + 2\eta\alpha\xi[\partial_\xi g_2(\eta,y)] - \partial_\xi a,\end{aligned} \tag{32}$$

$$\begin{aligned}\partial_\xi^2 G(\eta,y) = {} & -\frac{\eta\alpha}{2\xi}[1 + g_2(\eta,y)] + 2\eta\alpha[\partial_\xi g_2(\eta,y)] \\ & + 2\eta\alpha\xi[\partial_\xi^2 g_2(\eta,y)] - \partial_\xi^2 a,\end{aligned} \tag{33}$$

$$\partial_\xi g_2(\eta,y) = -\frac{1}{y}\int_0^\infty x\,dx\,\partial_\xi F(\eta,y)\ln\left|\frac{y+x}{y-x}\right|, \tag{34}$$

$$\partial_\xi^2 g_2(\eta,y) = -\frac{1}{y}\int_0^\infty x\,dx\,\partial_\xi^2 F(\eta,y)\ln\left|\frac{y+x}{y-x}\right|, \tag{35}$$

$$\partial_\xi F(\eta,y) = \frac{-1}{2[1+\cosh G(\eta,y)]}\partial_\xi G(\eta,y), \tag{36}$$

$$\begin{aligned}\partial_\xi^2 F(\eta,y) = {} & \frac{\sinh G(\eta,y)}{2[1+\cosh G(\eta,y)]^2}[\partial_\xi G(\eta,y)]^2 \\ & + \frac{-1}{2[1+\cosh G(\eta,y)]}\partial_\xi^2 G(\eta,y),\end{aligned} \tag{37}$$

where we use two constraints to fix $\partial_\xi a$ and $\partial_\xi^2 a$:

$$\int_0^\infty x^2 dx\,\partial_\xi F(\eta,x) = 0, \tag{38}$$

$$\int_0^\infty x^2 dx\,\partial_\xi^2 F(\eta,x) = 0. \tag{39}$$

We can easily see that results of GR are obtained by letting $\alpha = 0$ in the above formulas [Eqs. (13)–(39)] and solving them self-consistently. That is, GR's results are independent of α, while our results depend very much on α. Below, we will reproduce their results to compare them with our results.

Figure 1 shows plots of (a) $\widehat{E}_x(n,t)$, (b) $\widehat{V}_x(n,t)$, and (c) $\widehat{K}_x(n,t)$ as a function of t=ξ^{-1}. This figure can be classified into three groups from the convergence at large t. The lowest group is (a) $\widehat{E}_x(n,t)$, the next one is (b) $\widehat{V}_x(n,t)$, and the topmost corresponds to (c) $\widehat{K}_x(n,t)$. The curve with filled squares (results for α=0) in each group is that of GR. In each group when shown at t=1, curves for nonzero α represent α=0.1, 0.3, 0.5, 0.7, 0.8, and 0.9 in increasing order. Note that values of all curves approach 1 at $t \to 0$ since $F(\eta,k)$ becomes $\theta(k_F - k)$ at zero temperature. We see much difference between our results (corresponding to nonzero α) and those of GR over ranges of ~0.25 to ~1.25 in reduced temperature t. Note that for larger α, the difference becomes bigger. Especially, the second derivatives $\widehat{K}_x$ show a very distinctive behavior; (i) our values of $\widehat{K}_x$ increase less slowly to t~0.4 than GR's results but (ii) for larger α they increase much further to a maximum, while in this region GR's results decrease. For larger values of t ($\to\infty$), our results become the same as those of GR, from which we may say that at high temperatures the effects of self-energy corrections become less effective.

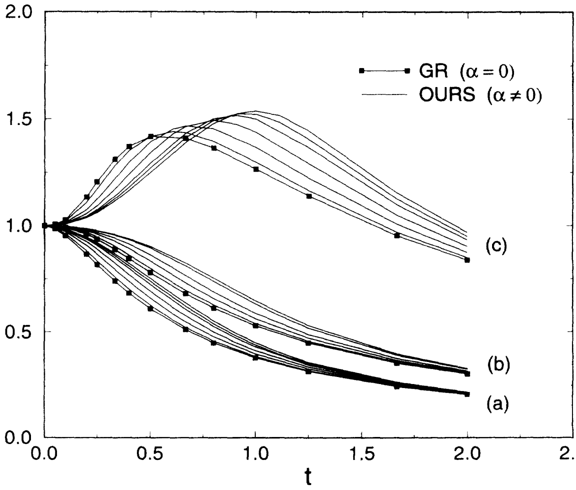

FIG. 1. Plot of group (a) $\widehat{E}_x(n,t)$, group (b) $\widehat{V}_x(n,t)$, and group (c) $\widehat{K}_x(n,t)$ as a function of t=ξ^{-1}. The GR's results with filled squares (corresponding to α=0) are independent of α, while ours are much dependent on α. For each group, results for α=0.0, 0.1, 0.3, 0.5, 0.7, 0.8, 0.9 (r_s=0.0, 0.60, 1.81, 3.01, 4.22, 4.82, 5.43) are shown in increasing order. The second derivatives $\widehat{K}_x$ show a distinctive behavior as α increases.

It is worth considering the behavior of $\widehat{E}_x(n,t)$, $\widehat{V}_x(n,t)$, and $\widehat{K}_x(n,t)$ at small t. That is, what is the first term in the power series in t? How does its coefficient depend on α?

For α=0 and $t \to 0$, the limiting behaviors are known:[4,8]

$$\widehat{E}_x(n,t) \sim 1 + \frac{\pi^2}{6} t^2 \ln t + A t^2, \tag{40}$$

$$\widehat{V}_x(n,t) \sim 1 - \frac{\pi^2}{12} t^2, \tag{41}$$

$$\widehat{K}_x(n,t) \sim 1 + \frac{\pi^2}{4} t^2, \tag{42}$$

where A is some known constant (A=0.767 409...). Note that terms containing A in the last two expressions cancel out each other. This value of A was calculated by Wasserman, Buckholtz, and DeWitt.[4] But they did not correct for the change in the chemical potential which is $-\pi^2/6$.[23] So one should get

$$A' = A - \pi^2/6 = -0.877\,525\ldots. \tag{43}$$

This value is also confirmed by numerical calculations at small t. In Fig. 2 (a), the filled circles, squares, and diamonds are numerical data points for $\widehat{E}_x$, $\widehat{V}_x$, and $\widehat{K}_x$, respectively. The lines are analytical ones given by Eqs. (40)–(43). The lowest solid line used the value of A' instead of A, while the dashed one used A. The line using A' fits our data very well.

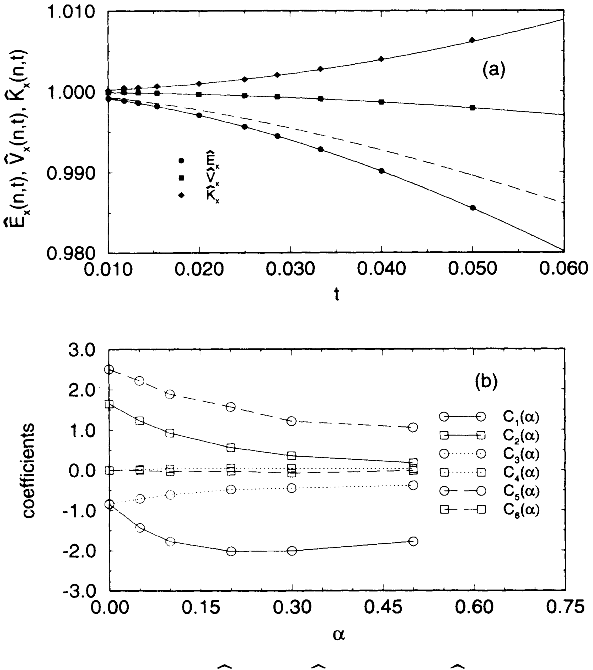

FIG. 2. (a) Plot of $\widehat{E}_x(n,t)$, $\widehat{V}_x(n,t)$, and $\widehat{K}_x(n,t)$ at small t for α=0. The filled symbols represent numerical data points, while the curves are given by analytical limiting behaviors. The lowest solid line used the value of A' instead of A. The dashed line using A is also shown for comparison. (b) The dependence of coefficients $C_1(\alpha), \ldots, C_6(\alpha)$ on α. Note that only $C_1(\alpha)$ increases from its α=0 value in magnitude and that $C_4(\alpha)$, $C_6(\alpha)$ are close to zero.

For nonzero α, we assume that $\widehat{E}_x(n,t)$ has a form of

$$\widehat{E}_x(n,t) \sim 1 + C_1(\alpha) t^2 + C_2(\alpha) t^2 \ln t. \tag{44}$$

Then we find the dependence of $\widehat{V}_x(n,t)$ and $\widehat{K}_x(n,t)$ at small t:

$$\widehat{V}_x(n,t) \sim 1 + C_3(\alpha) t^2 + C_4(\alpha) t^2 \ln t, \tag{45}$$

$$\widehat{K}_x(n,t) \sim 1 + C_5(\alpha) t^2 + C_6(\alpha) t^2 \ln t, \tag{46}$$

where the coefficients $C_3, \ldots, C_6$ are simply related to C_1 and C_2 by relations between $\widehat{V}_x$, $\widehat{K}_x$, and $\widehat{E}_x$.

Fitting numerical data to the above functions gives the dependence of coefficients on α, which is shown in Fig. 2 (b). For α=0, we set C_4 and C_6 to be zero and data fitting shows that fitted coefficients are close to analytical ones within a few percent. For example, we obtained $C_1(0)=-0.838\,643$, which is very close to $A'=-0.877\,525$. For nonzero α, the coefficients $C_4(\alpha)$, $C_6(\alpha)$ are close to zero, from which we may say that the terms proportional to $t^2 \ln t$ have a small contribution compared to t^2 terms, in $\widehat{V}_x$ and $\widehat{K}_x$. As α increases, the magnitude of every coefficient decreases from its α=0 value except $C_1(\alpha)$.

III. APPLICATION : PARAMAGNETIC SUSCEPTIBILITY

The function $K_x(n,T)$ can be used in the study of the temperature-dependent paramagnetic susceptibility $\chi_p(n,t)$ of an interacting electron gas. The long wavelength ($q \to 0$) limit of $\chi_p(n,t)$ in the static case (ω=0)[8,22] is

$$\chi_p(n,t)_{q\to 0} = -g^2 \mu_B^2 \frac{\chi_0(n,t)_{q\to 0}}{1 - K_x(n,T)\chi_0(n,t)_{q\to 0}}, \tag{47}$$

where $g \simeq 2$ is the electron g factor and μ_B is the usual Bohr magneton. In the limit of $q \to 0$, $\chi_0(n,t)$, the Lindhard susceptibility at finite temperature, becomes a simple form:

$$\chi_0(n,t)_{q\to 0} = -\frac{1}{\pi^3 e^2 a_B^2} \frac{h(t)}{\alpha}, \tag{48}$$

$$h(t) = \int_0^\infty dx\, f(x), \tag{49}$$

$$f(x) = 1/(\exp[\xi x^2 - \beta\mu] + 1). \tag{50}$$

Note that the noninteracting occupation number $f(x)$ can be obtained by putting η=1 and α=0 in $F(\eta,x)$. For some comments on the Lindhard susceptibility, see Appendix B.

First, it is worth noting the result of the zero-temperature paramagnetic susceptibility:

$$\begin{aligned}\chi_p(n,0)_{q\to 0} &= -g^2 \mu_B^2 \frac{\chi_0(n,0)_{q\to 0}}{1 - K_x(n,0)\chi_0(n,0)_{q\to 0}} \\ &= g^2 \mu_B^2 \frac{1}{\pi^3 e^2 a_B^2 \alpha} \frac{1}{1-\alpha}.\end{aligned} \tag{51}$$

This expression shows the well-known zero temperature instability point α=1, i.e., r_s=6.029, of the paramagnetic state.

Define $\widetilde{\chi}_p(n,t)$ as a function of α at given t:

$$\widetilde{\chi}_p(n,t) = \frac{\chi_p(n,t)_{q\to 0}}{g^2\mu_B^2/\pi^3 e^2 a_B^2} = \frac{1}{\alpha}\frac{h(t)}{1-\alpha h(t)\widehat{K}_x(n,t)}. \tag{52}$$

To compare our results with GR's, the following equation is used in drawing figures:

$$\widetilde{\chi}_p(n,t) = \frac{1}{r_s}\frac{h(t)}{1-\alpha h(t)\widehat{K}_x(n,t)}. \tag{53}$$

Figure 3 shows plots of $\widetilde{\chi}_p(n,t)$, where curves with filled circles represent our results and curves without symbols represent those of GR. From Figs. 3(a) to 3(f), the results for α=0.1, 0.3, 0.5, 0.7, 0.8, and 0.9 are shown.

In Fig. 3 (a) for α=0.1, two results are (almost) the same as each other. As α increases, our $\widetilde{\chi}_p(n,t)$ becomes much different from theirs. It is due to the fact that, in the denominator of $\widetilde{\chi}_p(n,t)$, our $\widehat{K}_x(n,t)$ for larger α is much different from that of GR. Their results show that $\widetilde{\chi}_p(n,t)$ rises above its zero-temperature value at small t, goes through a peak, and then decreases rapidly with increasing t. This behavior is more outstanding in larger α than in smaller α. Finally, their values of $\widetilde{\chi}_p(n,t)$ become negative at some larger α (say, α=0.9) over $t\sim 0.23$ to $\sim$0.48. But our results are quite different from theirs: (i) $\widetilde{\chi}_p(n,t)$ starts to decrease at small t for all α; (ii) $\widetilde{\chi}_p$ does not show a peak but always decreases with increasing t; and (iii) our results do not become negative even at α=0.9, while their results show an instability.

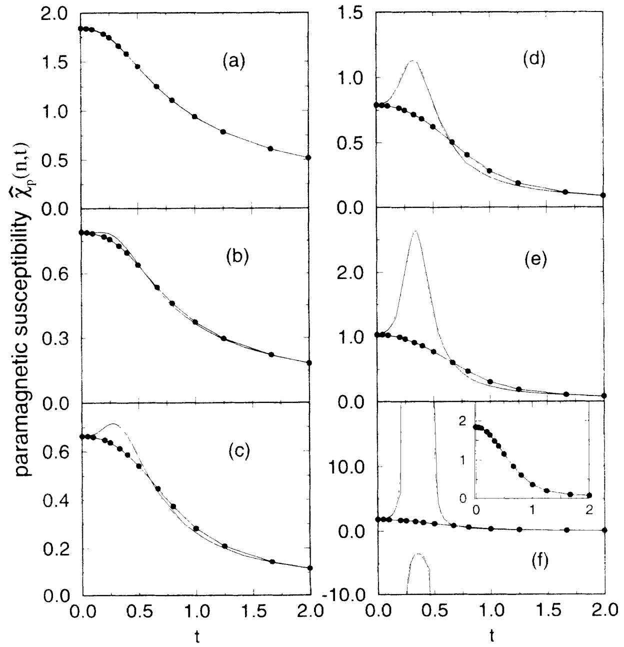

FIG. 3. Plot of $\widetilde{\chi}_p(n,t)$, where curves with filled circles and those without symbols represent our results and GR's, respectively: (a) α=0.1, (b) 0.3, (c) 0.5, (d) 0.7, (e) 0.8, and (f) 0.9. In (a), two results are shown to be the same. As α increases, our results become much different from those of GR. For given α, our $\widetilde{\chi}_p(n,t)$ does not show any peak but always decreases with increasing t. Note an instability of GR shown in (f), while our system is still stable. Inset in (f): better view of our result for α=0.9.

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APPENDIX A: NOTES ON THE THERMODYNAMIC POTENTIAL

At nonzero temperatures it is best to employ the finite-temperature formulation[13] of Matsubara. In this method the following equations give the Hamiltonian of the electron gas and the expression for the thermodynamic potential Ω.

$$H = H_0 + V, \tag{A1}$$

$$H_0 = \sum_{\mathbf{p}\sigma} \xi_{\mathbf{p}} c^{\dagger}_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma}, \tag{A2}$$

$$V = \frac{1}{2\nu}\sum_{\mathbf{q}\neq 0} v_{\mathbf{q}} \sum_{\mathbf{kp}s\sigma} c^{\dagger}_{\mathbf{k+q},s} c^{\dagger}_{\mathbf{p-q},\sigma} c_{\mathbf{p}\sigma} c_{\mathbf{k}s}, \tag{A3}$$

$$\beta\Omega = \beta\Omega_0 - \sum_l U_l, \tag{A4}$$

$$\beta\Omega_0 = \sum_{\mathbf{p}\sigma} \ln[1 + e^{-\beta\xi_{\mathbf{p}}}], \tag{A5}$$

$$U_l = \frac{(-1)^l}{l}\int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_l \langle T_\tau V(\tau_1)\cdots V(\tau_l)\rangle. \tag{A6}$$

The energy with respect to the chemical potential is $\xi_{\mathbf{p}} = \hbar^2 p^2/2m - \mu$, while $v_{\mathbf{q}} = 4\pi e^2/q^2$ in three dimensions. In the last expression, the τ dependence of the interaction is evaluated in the interaction representation, and only different connected diagrams are evaluated.

The lowest level of approximation, under the title of "Hartree-Fock" (HF), is to consider only the single diagram shown in Fig. 4(a). It is simply

$$\begin{aligned} U_1 &= -\beta\langle V\rangle \\ &= -\frac{1}{2\nu}\sum_{\mathbf{pq}\sigma} v_{\mathbf{q}} n_{\mathbf{p}} n_{\mathbf{p+q}} \\ &= \frac{1}{2}\sum_{\mathbf{p}\sigma} n_{\mathbf{p}}\Sigma_x(p), \end{aligned} \tag{A7}$$

$$\Sigma_x(p) = -\frac{1}{\nu}\sum_{\mathbf{q}} v_{\mathbf{q}} n_{\mathbf{p+q}}, \tag{A8}$$

$$n_{\mathbf{p}} = \frac{1}{e^{\beta\xi_{\mathbf{p}}}+1}. \tag{A9}$$

The Hartree-Fock exchange energy is calculated using only the first term U_1, which is the same as E_g. In this level of approximation, the occupation numbers $n_{\mathbf{p}}$ of

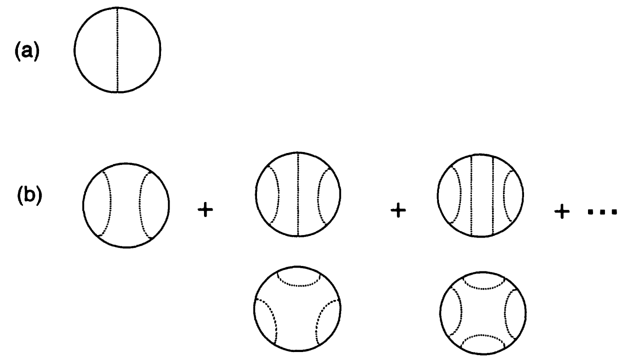

FIG. 4. One-bubble diagrams for evaluating the thermodynamic potential Ω_x. The solid lines represent the unperturbed electron Green's functions, while the dotted ones represent Coulomb interactions $v_{\mathbf{q}}=4\pi e^2/q^2$. (a) First-order diagram for HFA and (b) higher-order diagrams for corrections.

the electrons are those of the noninteracting electron gas. This expression was discussed in detail at nonzero temperatures by GR[8] using the density-functional approach.

The next level of approximation, in HF, is to sum the diagrams shown in Fig. 4(b) and add them to the above term. To do this and do more generally, we follow a simple argument by Luttinger and Ward.[14] The prescription for computing Ω is to take each possible closed linked diagram that can be drawn just once. Suppose we consider any lth order diagram for Ω. If we break open any of its $2l$ lines we obtain a possible lth order diagram for the Green's function. Let us call $\Sigma_l(p)$ the total self-energy part of the lth order, proper or improper. Note that we get the same closed linked diagram $2l$ times when we close all possible lth order Green's function diagrams. Then we may obtain the following expression for Ω_l, the lth order contribution of Ω, summed over spin:

$$\Omega_l = \frac{1}{\beta}\sum_{\mathbf{p},ip_n}\frac{1}{l}\mathcal{G}^{(0)}(p)\Sigma_l(p), \tag{A10}$$

where $\mathcal{G}^{(0)}$ is the unperturbed Green's function. After some manipulations, we obtain

$$\Omega - \Omega_0 = \frac{1}{\beta}\sum_{\mathbf{p},ip_n}\int_0^1\frac{d\eta}{\eta}\mathcal{G}(\eta,p)\Sigma(\eta,p), \tag{A11}$$

where $\mathcal{G}$ is the Matsubara Green's function with the self-energy Σ.

The proof of this expression is given in Abrisokov *et al.*[15] and a simple treatment for electron-phonon systems is also shown in Mahan.[13] Using the exchange self-energy Σ_x and the Green's function $\mathcal{G}^{(x)}$ in Eq. (A11), we obtain the Hartree-Fock thermodynamic potential $\Omega_x=\nu E_x$.

APPENDIX B: NOTES ON THE LINDHARD SUSCEPTIBILITY

In Sec. II, we evaluated $K_x(n,T)$ using a formalism with a full self-consistency. Here K_x is the LDA version of the Hubbard local-field correction,[1,24] usually called $G(q)$; more precisely, $K_x=-v_{\mathbf{q}}G(q)$ at $q\rightarrow 0$.[20] To give the self-consistency to the evaluation of the paramagnetic susceptibility $\chi_P(n,t)$, we need to determine what is appropriate for the place of the Lindhard susceptibility in Eq. (47). Note that if we only include ladder diagrams for a single bubble, the polarization $P_x(q)$ and the paramagnetic susceptibility χ_P is the same up to a constant $(-g^2\mu_B^2)$. If only exchange effects are considered, we are actually considering only a single bubble. Thus, the formula $\chi_P(n,t) = -g^2\mu_B^2P_x(q)$ is justified in the HF level.

First candidate is still to use the Lindhard susceptibility,

$$\begin{aligned}\chi_0(n,t)_{q\rightarrow 0} &= \lim_{q\rightarrow 0}\frac{2}{\beta\nu}\sum_{\mathbf{p},ip_n}\mathcal{G}^{(0)}(p)\mathcal{G}^{(0)}(p+q)\\ &= \lim_{q\rightarrow 0}\frac{2}{\nu}\sum_{\mathbf{p}}\frac{n_{\mathbf{p}}-n_{\mathbf{p+q}}}{\xi_{\mathbf{p}}-\xi_{\mathbf{p+q}}}\\ &= \frac{-1}{\pi^3e^2a_B^2}\frac{h(t)}{\alpha},\end{aligned} \tag{B1}$$

$$h(t) = \int_0^\infty dx\, f(x). \tag{B2}$$

Second one is to use $H(t)$ instead of $h(t)$,

$$H(t) = \int_0^\infty dx\, F(x), \tag{B3}$$

where $F(x)$ is obtained by putting η=1 in $F(\eta,x)$, i.e., $F(x) \equiv F(\eta{=}1,x)$. For $H(t)$ with nonzero α, the occupation number $F(x)$ is for the interacting gas rather than for noninteracting gas, as in Niklasson.[25] Using interacting occupation numbers means that one is using, in an approximate fashion, interacting Green's functions for internal lines in the bubble. That is,

$$\begin{aligned}\chi_0^H(n,t)_{q\rightarrow 0} &= \lim_{q\rightarrow 0}\frac{2}{\nu}\sum_{\mathbf{p}}\frac{F(p)-F(|\mathbf{p}+\mathbf{q}|)}{\xi_{\mathbf{p}}-\xi_{\mathbf{p+q}}}\\ &= \frac{-1}{\pi^3e^2a_B^2}\frac{H(t)}{\alpha}.\end{aligned} \tag{B4}$$

Third choice is to use fully dressed Green's functions for internal lines:

$$\begin{aligned}\chi_0^F(n,t)_{q\rightarrow 0} &= \lim_{q\rightarrow 0}\frac{2}{\beta\nu}\sum_{\mathbf{p},ip_n}\mathcal{G}^{(x)}(p)\mathcal{G}^{(x)}(p+q)\\ &= \lim_{q\rightarrow 0}\frac{2}{\nu}\sum_{\mathbf{p}}\frac{F(p)-F(|\mathbf{p}+\mathbf{q}|)}{E(p)-E(|\mathbf{p}+\mathbf{q}|)},\end{aligned} \tag{B5}$$

where $E(p) = \xi_{\mathbf{p}} + \Sigma_x(p)$.

Originally Hubbard,[24] in his formalism on the polarization, used χ_0 instead of χ_0^F, while a derivation[1] using the equation-of-motion method shows that χ_0^F is correct. The LDA version of the Hubbard correction was first derived by Hedin and Lundqvist,[26] who used χ_0. Niklasson[25] used χ_0^H instead of χ_0 in his Lindhard susceptibility and Schweng and Böhm[27] defined a generalized Lindhard function with the same spirit of Niklasson. Rajagopal *et al.*[8,22,28] used it differently in their several papers. In earlier work,[28] fully dressed Green's functions were used to give χ_0^F. In the next one,[22] Rajagopal used $E(k) = \xi_k + V_x$, where $V_x = \Sigma_x(k_F)$ at $T\rightarrow 0$. Using this $E(k)$ is not one of three choices mentioned above. In another one,[8] of which scheme we follow, they used $E(k) = \xi_k$ and thus χ_0.

Anyway, the third choice using fully dressed Green's functions seems to be right among three possibilities. But unfortunately this seemingly exact way fails because the fully dressed Lindhard susceptibility $\chi^F_{0,q\to 0}$ becomes zero at $T \to 0$ due to divergence of the inverse effective mass:

$$\begin{aligned}\chi_0^F(n,t)_{q\to 0} &= \frac{2}{\nu}\sum_{\mathbf{p}} \frac{\partial F(p)}{\partial E(p)} \\ &= \frac{k_F^3}{2\pi^2}\int_0^\infty y^2 dy \frac{1}{\frac{\partial E(y)}{\partial y}} \frac{\partial F(y)}{\partial y}. \qquad \text{(B6)}\end{aligned}$$

Here, at $T \to 0$, $F(y) \to \theta(1-y)$ and $\frac{\partial F(y)}{\partial y} \to \delta(1)$, and then

$$\left.\frac{\partial E(y)}{\partial y}\right|_{y=1} \propto 1/m^* \to \infty. \qquad \text{(B7)}$$

Therefore, $\chi^F_{0,q\to 0} \to 0$ at $T \to 0$. Thus we get the zero value of the paramagnetic susceptibility. By the conserving approximation[29–32] in the level of HF, we find a standard Hartree-Fock result:

$$P_x(0) = \frac{-1}{\pi^3 e^2 a_B^2}\frac{1}{\alpha}\frac{1}{1-\alpha} \qquad \text{(B8)}$$

in the limit of $T \to 0$. We should have found a finite value of the zero-temperature paramagnetic susceptibility. Therefore, the third way should be thrown away.

Two other choices give the exact value in the limit of $T \to 0$ as in the conserving approximation. The second one is using interacting occupation numbers with self-energy corrections only in the numerator, while it does not give any self-energy correction to the denominator. Thus it appears less consistent than using noninteracting things in both denominator and numerator in the Lindhard function. Here we claim that the first choice may be correct. This argument will be clarified elsewhere[32] by comparing present results with those from conserving approximations.

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