PHYSICAL REVIEW B VOLUME 51, NUMBER 24 15 JUNE 1995-II

Spin-polarized Hartree-Fock approximation at nonzero temperatures

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(Received 14 September 1994; revised manuscript received 17 January 1995)

The Hartree-Fock exchange energy is calculated for the spin-polarized electron gas at nonzero temperatures. This calculation is done self-consistently in that the Hartree-Fock self-energy is included self-consistently in the Fermi-Dirac occupation numbers while performing a coupling constant integral. The internal energy and entropy are also considered. We calculate the first and second derivatives of the exchange energy, internal energy, and entropy with respect to number density and/or spin polarization density, which are used for calculations of response functions such as the compressibility and polarization. One should have in mind that our exchange-only scheme using the coupling-constant-integral formalism is different from the usual Hartree-Fock approximation at nonzero temperatures and is indeed its self-consistent generalization.

I. INTRODUCTION

Electron-electron interactions play a central role in metal physics, and the homogeneous electron gas[1] is the standard model in which to investigate these interactions. The positive charges are spread uniformly throughout the sample and the difficult problems are due to electron-electron interactions. In this model, the direct Coulomb energy becomes zero so that the net system is charge neutral. The lowest level of approximation is therefore to include only electron exchange, which is called the Hartree-Fock approximation (HFA). In the approximation, the spin-polarized Hartree-Fock (HF) exchange energy is given by

$$E_g = -\frac{1}{2\nu}\sum_{\mathbf{pq}\sigma} v_{\mathbf{q}} n_{\mathbf{p}\sigma} n_{\mathbf{p+q}\sigma}, \tag{1}$$

where $v_{\mathbf{q}} = 4\pi e^2/q^2$ in three dimensions is spin independent, ν is the volume, and the spin index σ is $\pm$ for up and down spin, respectively. At zero temperature, the Fermi-Dirac occupation functions are $n_{\mathbf{p}\sigma} = \theta(k_\sigma - p)$, a step function at a wave vector k_σ, which corresponds to the Fermi wave vector k_F in the paramagnetic case. That is, spin-up electrons occupy each one-electron level with $k < k_+$, and spin-down electrons, each with $k < k_-$. In the paramagnetic system, we do not have to consider spins explicitly, which means that spin summations can be replaced by a factor of 2 and k_σ becomes the Fermi wave vector k_F. Here, we wish to consider spins explicitly and evaluate the spin-polarized HF exchange energy at nonzero temperatures.

The finite-temperature formalism of the local-density approximation was formally set up by Mermin[2] long ago. Only a few generalizations have been reported so far.[3–7] Gupta and Rajagopal[3] proposed an exchange-only scheme for the paramagnetic system, which was generalized in the self-consistent way by the present authors[7] (to be referred to as HM). Kanhere *et al.*[6] extended calculations of Gupta and Rajagopal[3,4] to the spin-polarized case. Previously,[7] we evaluated the HF exchange energy self-consistently by including the self-energy $\Sigma_x(p)$ in the argument of the occupation numbers, while performing a coupling constant integral.[8–10] We used the correct Fermi-Dirac function $F(p) = 1/\{\exp[\beta E(p)] + 1\}$, with $E(p) = \varepsilon_{\mathbf{p}} + \Sigma_x(p) - \mu$, where $\beta = 1/k_B T$, $\varepsilon_{\mathbf{p}} = \hbar^2 p^2/2m$, and μ is the chemical potential. A factor of 2 was multiplied where it was needed, instead of considering explicit spin summations.

We wish to extend the previous works of HM to the spin-polarized case. This extension is, within the exchange-only scheme, equivalent to extension of works by Kanhere *et al.*,[6] using our coupling-constant-integral formalism,[7] and also equivalent to generalization of the zero-temperature formalism by Gunnarsson and Lundqvist[11] to the nonzero-temperature one. On the other hand, it is worth noting that a Green function theory of the itinerant spin-polarized electron gas at $T = 0$ was published in Ref. 12, where the ground state and excited state properties of the spin-polarized HF electron gas were studied in some detail. Rajagopal *et al.*[12] also studied a treatment of the integral equation of the vertex function at $T = 0$, which includes the importance of the correct self-energy. In a way, the present authors reexamine this problem for $T \neq 0$. It is also worthwhile to note

0163-1829/95/51(24)/17417(14)/$06.00

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that Dandrea *et al.*[13] studied the unpolarized electron gas at any degeneracy for $T \neq 0$.

The aim of this paper is to generalize the previous formalism of HM by considering spin expressions explicitly. Actually, Eq. (1) is the correct result only in the first order of perturbation theory, so we wish to include higher-order terms in the perturbation theory. To do this, we express the spin-polarized HF exchange energy $\Omega_x(n,s,T)$ as an integral over the coupling constant, with the spin-dependent Fermi-Dirac function $F_\sigma(p)$ including the self-energy $\Sigma_{x\sigma}(p)$ in its argument:

$$F_\sigma(p) = \frac{1}{e^{\beta E_\sigma(p)} + 1}, \tag{2}$$

where $E_\sigma(p) = \varepsilon_{\mathbf{p}} + \Sigma_{x\sigma}(p) - \mu_\sigma$, μ_σ being the chemical potential for spin σ. Above, n is the number density and s is the spin-polarization density. In Sec. II, the nonzero-temperature formalism calculating the exchange energy $E_x(n,s,T)$ and its derivatives with respect to number density and/or spin-polarization density is developed. The internal energy, entropy, and their derivatives with respect to density are also considered. In Sec. III, some applications are considered in calculating the energies, potentials, and response functions such as the compressibility and polarization. In Sec. IV, the present work is summarized and our exchange-only scheme using the coupling-constant-integral formalism is compared with the usual HFA in the viewpoint of the kinetic part of the exchange-correlation energy, $T_{\rm xc}$. In the Appendixes, some comments are made on the chemical potential and the Seitz theorem, and a simple generalization of $T_{\rm xc}$ to the nonzero-temperature case is also discussed.

II. THEORY: TEMPERATURE DEPENDENCE OF THE SPIN-POLARIZED HFA

We consider a homogeneous spin-polarized electron gas without external potential. The Hartree potential of electron gas is canceled by charge neutrality. In this paper, we consider only exchange effects, neglecting correlation processes. 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 HF exchange energy per volume $E_x(n,s,T) \equiv \Omega_x(n,s,T)/\nu$ is given by an integral over the coupling constant η:

$$E_x(n,s,T) = \sum_\sigma E_{x\sigma}(n_\sigma,T), \tag{3}$$

$$E_{x\sigma}(n_\sigma,T) = \frac{1}{2\beta\nu} \sum_{\mathbf{p},ip_n} \int_0^1 \frac{d\eta}{\eta} \Sigma_{x\sigma}(\eta,p) \mathcal{G}_\sigma^{(x)}(\eta,p), \tag{4}$$

where n is the number density,

$$n = \frac{k_F^3}{3\pi^2} = n_+ + n_- = \frac{k_+^3}{6\pi^2} + \frac{k_-^3}{6\pi^2}, \tag{5}$$

and s is the spin-polarization density, which will be defined below, and $\mathcal{G}_\sigma^{(x)}$ is the fully dressed Matsubara Green's function with the exchange self-energy $\Sigma_{x\sigma}$, σ being $\pm$ for up and down spin,

$$\mathcal{G}_\sigma^{(x)}(\eta,p) = \frac{1}{ip_n - [\varepsilon_{\mathbf{p}} + \Sigma_{x\sigma}(\eta,p) - \mu_\sigma]}, \tag{6}$$

$$\Sigma_{x\sigma}(\eta,p) = -\frac{1}{\beta\nu} \sum_{\mathbf{k},ik_n} \eta v_{\mathbf{p}-\mathbf{k}} \mathcal{G}_\sigma^{(x)}(\eta,k). \tag{7}$$

The decoupling of up- and down-spin components comes from the fact that bare (unscreened) Coulomb interactions $v_{\mathbf{q}} = 4\pi e^2/q^2$ are independent of spin.

If we assumed that every occupied one-electron level would be occupied by two electrons of opposite spin, it would give the previous results of HM for the paramagnetic case.[7] A more general possibility, leading to a net spin imbalance, would be to fill each one-electron level with $k < k_+$ with spin-up electrons, and each with $k < k_-$ with spin-down electrons. In that case, the system would have a nonvanishing magnetization density,

$$M = -g\mu_B(n_+ - n_-), \tag{8}$$

where $g \simeq 2$ is the electron g factor, and μ_B is the usual Bohr magneton. For convenience, we define the spin-polarization density s, and the ratio ζ of the spin-polarization density to the number density:

$$s = n\zeta = \frac{\zeta k_F^3}{3\pi^2} = n_+ - n_- = \frac{k_+^3}{6\pi^2} - \frac{k_-^3}{6\pi^2}, \tag{9}$$

and then we obtain

$$n_\sigma = \frac{1}{2}(n + \sigma s) = \frac{n}{2}(1 + \sigma\zeta). \tag{10}$$

Due to spins' decoupling, the formalism below is almost the same as in the previous paper by HM, except for the spin index. That is, if the spin index σ is dropped out for spin components considered, almost all formulas are the same as the previous ones. For example, dropping σ out in Eqs. (6) and (7) directly gives the paramagnetic Green's function and self-energy. Since the exchange self-energy [Eq. (7)] does not depend upon the energy variable ip_n, the frequency summation of the Green's function $\mathcal{G}_\sigma^{(x)}$ just gives the occupation number $F_\sigma(\eta,p) = 1/\{\exp[\beta E_\sigma(\eta,p)] + 1\}$. Then,

$$E_{x\sigma}(n_\sigma,T) = \frac{1}{2\nu} \sum_{\mathbf{p}} \int_0^1 \frac{d\eta}{\eta} \Sigma_{x\sigma}(\eta,p) F_\sigma(\eta,p), \tag{11}$$

$$\begin{aligned} \Sigma_{x\sigma}(\eta,p) &= -\int \frac{d^3k}{(2\pi)^3} \eta v_{\mathbf{p}-\mathbf{k}} F_\sigma(\eta,k), \\ &= -\frac{\eta e^2}{\pi p} \int_0^\infty \frac{k\,dk}{e^{G_\sigma(\eta,k)} + 1} \ln\left|\frac{p+k}{p-k}\right|, \end{aligned} \tag{12}$$

$$G_\sigma(\eta,k) = \beta E_\sigma(\eta,k) = \beta[\varepsilon_{\mathbf{k}} + \Sigma_{x\sigma}(\eta,k) - \mu_\sigma], \tag{13}$$

$$\mu_\sigma = \frac{\hbar^2 k_\sigma^2}{2m} - \frac{\eta e^2 k_\sigma}{\pi} + \delta\mu_\sigma, \tag{14}$$

$$\mu_\sigma^0 = \frac{\hbar^2 k_\sigma^2}{2m}. \tag{15}$$

Here, μ_σ^0 is a sort of the Fermi energy corresponding to k_σ, $-\eta e^2 k_\sigma/\pi$ is zero-temperature shift in the chemical potential, due to the exchange self-energy of spin σ, and $\delta\mu_\sigma$ is nonzero temperature deviation in the chemical potential. Note that Eqs. (12) and (13) provide the self-consistent equations for $\Sigma_{x\sigma}$, G_σ, and F_σ.[14,15]

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

$$\xi = \frac{\mu^0}{k_B T} = t^{-1}, \tag{16}$$

$$\alpha = \frac{1}{\pi a_B k_F} = \frac{r_s}{(4/9\pi^4)^{1/3}} = \frac{r_s}{6.029}, \tag{17}$$

where a_B is the Bohr radius, and r_s is an effective radius, which comes from $n^{-1} = 4\pi(r_s a_B)^3/3$. Thus, α (or r_s) is small for a high-density electron gas and large for a low-density one. For the spin-polarized system, we need more parameters:

$$\xi_\sigma = \frac{\mu^0_\sigma}{k_B T} = t_\sigma^{-1}, \tag{18}$$

$$\alpha_\sigma = \frac{1}{\pi a_B k_\sigma}. \tag{19}$$

From Eqs. (5) and (9), we obtain the relations

$$k_\sigma = k_F(1+\sigma\zeta)^{1/3}, \tag{20}$$

$$\alpha_\sigma = \alpha(1+\sigma\zeta)^{-1/3}, \tag{21}$$

$$\xi_\sigma = \xi(1+\sigma\zeta)^{2/3}. \tag{22}$$

Scaling all momenta by k_σ, we obtain

$$G_\sigma(\eta,y) = \beta E_\sigma(\eta,y) = G_{1\sigma}(\eta,y) + G_{2\sigma}(\eta,y), \tag{23}$$

$$G_{1\sigma}(\eta,y) = \beta(\varepsilon_{\mathbf{k}} - \mu_\sigma) = \xi_\sigma g_{1\sigma}(\eta,y) - a_\sigma, \tag{24}$$

$$g_{1\sigma}(\eta,y) = y^2 - 1 + 2\eta\alpha_\sigma, \tag{25}$$

$$a_\sigma = \xi_\sigma \delta\mu_\sigma/\mu^0_\sigma, \tag{26}$$

$$G_{2\sigma}(\eta,y) = \beta\Sigma_{x\sigma}(\eta,y) = 2\eta\xi_\sigma\alpha_\sigma g_{2\sigma}(\eta,y), \tag{27}$$

$$g_{2\sigma}(\eta,y) = -\frac{1}{y}\int_0^\infty \frac{x\,dx}{e^{G_\sigma(\eta,x)}+1}\ln\left|\frac{y+x}{y-x}\right|. \tag{28}$$

The corrections of the chemical potential $\delta\mu_\sigma$ are determined by the number conservation $n = \frac{1}{\nu}\sum_{\mathbf{k}\sigma} F_\sigma(\eta,k)$, and the fixed value of the spin-polarization density $s = \frac{1}{\nu}\sum_{\mathbf{k}}(F_+ - F_-)$, which give the following condition for each spin σ:

$$\int_0^\infty x^2 dx F_\sigma(\eta,x) = \frac{1}{3}. \tag{29}$$

Given n and T, we wish to calculate the HF exchange energy and its derivatives with respect to density, when varying the value of s (i.e., ζ). By taking derivatives of $E_x(n,s,T)$ with respect to density, we define the exchange potential $V_x(n,s,T)$, the "interaction function" $K_x(n,s,T)$, etc., and their corresponding spin components, which appear in the calculation of response functions.[3,16] Following Ref. 16, in which the spin-density-functional (SDF) formalism is given, we obtain[17]

$$V_x(n,s,T) = \frac{\partial E_x(n,s,T)}{\partial n} = \frac{1}{2}\sum_\sigma \frac{dE_{x\sigma}(n_\sigma,T)}{dn_\sigma} \equiv \frac{1}{2}\sum_\sigma V_{x\sigma}(n_\sigma,T), \tag{30}$$

$$W_x(n,s,T) = \frac{\partial E_x(n,s,T)}{\partial s} = \frac{1}{2}\sum_\sigma \sigma\frac{dE_{x\sigma}(n_\sigma,T)}{dn_\sigma} \equiv \frac{1}{2}\sum_\sigma \sigma V_{x\sigma}(n_\sigma,T), \tag{31}$$

$$K_x(n,s,T) = \frac{\partial^2 E_x(n,s,T)}{\partial n^2} = \frac{1}{4}\sum_\sigma \frac{d^2E_{x\sigma}(n_\sigma,T)}{dn_\sigma^2} \equiv \frac{1}{4}\sum_\sigma K_{x\sigma}(n_\sigma,T), \tag{32}$$

$$G_x^{(1)}(n,s,T) = \frac{\partial^2 E_x(n,s,T)}{\partial n\partial s} = \frac{1}{4}\sum_\sigma \sigma\frac{d^2E_{x\sigma}(n_\sigma,T)}{dn_\sigma^2} \equiv \frac{1}{4}\sum_\sigma \sigma K_{x\sigma}(n_\sigma,T), \tag{33}$$

$$G_{x\perp}^{(2)}(n,s,T) = \frac{W_x(n,s,T)}{s} \equiv \frac{1}{2s}\sum_\sigma \sigma V_{x\sigma}(n_\sigma,T), \tag{34}$$

where the spin components will be useful below in expressing the formalism of response functions. For the spin components $E_{x\sigma}(n_\sigma,T)$, $V_{x\sigma}(n_\sigma,T)$, and $K_{x\sigma}(n_\sigma,T)$, we consider the normalized quantities to their zero-temperature values. For $E_{x\sigma}(n_\sigma,T)$, we have

$$\widehat{E}_{x\sigma}(n_\sigma,t_\sigma) = \frac{E_{x\sigma}(n_\sigma,T)}{E_{x\sigma}(n_\sigma,0)} = -2\int_0^1 d\eta\int_0^\infty dy\,y^2 g_{2\sigma}(\eta,y)F_\sigma(\eta,y), \tag{35}$$

$$E_{x\sigma}(n_\sigma,0) = -3e^2k_\sigma n_\sigma/4\pi = -e^2k_\sigma^4/8\pi^3. \tag{36}$$

Note that the integral $\widehat{E}_{x\sigma}(n_\sigma,t_\sigma)$ depends on the spin density n_σ only through $\xi_\sigma = t_\sigma^{-1}$. We may write down $\widehat{E}_{x\sigma}(n_\sigma,t_\sigma) = \widehat{E}_{x\sigma}(\xi_\sigma)$, and then

$$\widehat{V}_{x\sigma}(n_\sigma,t_\sigma) = \frac{V_{x\sigma}(n_\sigma,T)}{V_{x\sigma}(n_\sigma,0)} = \widehat{E}_{x\sigma} + \frac{\xi_\sigma}{2}\frac{d\widehat{E}_{x\sigma}}{d\xi_\sigma}, \tag{37}$$

$$V_{x\sigma}(n_\sigma,0) = -(e^2/\pi)(6\pi^2 n_\sigma)^{1/3}, \tag{38}$$

$$\widehat{K}_{x\sigma}(n_\sigma,t_\sigma) = \frac{K_{x\sigma}(n_\sigma,T)}{K_{x\sigma}(n_\sigma,0)} = \widehat{E}_{x\sigma} + \frac{7\xi_\sigma}{2}\frac{d\widehat{E}_{x\sigma}}{d\xi_\sigma} + \xi_\sigma^2\frac{d^2\widehat{E}_{x\sigma}}{d\xi_\sigma^2}, \tag{39}$$

$$K_{x\sigma}(n_\sigma,0) = -(e^2/3\pi)(6\pi^2)^{1/3}n_\sigma^{-2/3}. \tag{40}$$

Note that the procedure to obtain $\widehat{E}_{x\sigma}(n_\sigma,t_\sigma)$, $\widehat{V}_{x\sigma}(n_\sigma,t_\sigma)$, and $\widehat{K}_{x\sigma}(n_\sigma,t_\sigma)$ is exactly the same as that to obtain $\widehat{E}_x(n,t)$, $\widehat{V}_x(n,t)$ and $\widehat{K}_x(n,t)$ in the previous paper by HM, with only changes of $n \to n_\sigma$, $\xi \to \xi_\sigma$, $\alpha \to \alpha_\sigma$. That is, the behaviors of $\widehat{E}_{x\sigma}(n_\sigma,t_\sigma)$, $\widehat{V}_{x\sigma}(n_\sigma,t_\sigma)$, and $\widehat{K}_{x\sigma}(n_\sigma,t_\sigma)$ are exactly the same as those of corresponding functions in Fig. 1 of Ref. 7. The normalized functions $\widehat{E}_{x\sigma}$, $\widehat{V}_{x\sigma}$, and $\widehat{K}_{x\sigma}$ are shown for α=0.5 (r_s=3.01) in Fig. 1(a). If t_σ and n_σ are replaced by t and n, respectively, the normalized functions are the same as those in the paramagnetic case. They range over 0 to ~2; $\widehat{E}_{x\sigma}$ and $\widehat{V}_{x\sigma}$ decrease from their zero-temperature values, while $\widehat{K}_{x\sigma}$ increases from its zero-temperature value, goes through a bump, and then decreases with increasing t_σ.

In summary, for given n, s, and T, we can obtain ζ, k_σ, α_σ, and ξ_σ for each spin σ. With α_σ, ξ_σ, we obtain spin components $\widehat{E}_{x\sigma}$, $\widehat{V}_{x\sigma}$, and $\widehat{K}_{x\sigma}$. By summing over spin, $E_x(n,s,T), V_x(n,s,T),\ldots, G^{(2)}_{x\perp}(n,s,T)$ are obtained through Eqs. (3), (30),..., (34), respectively.

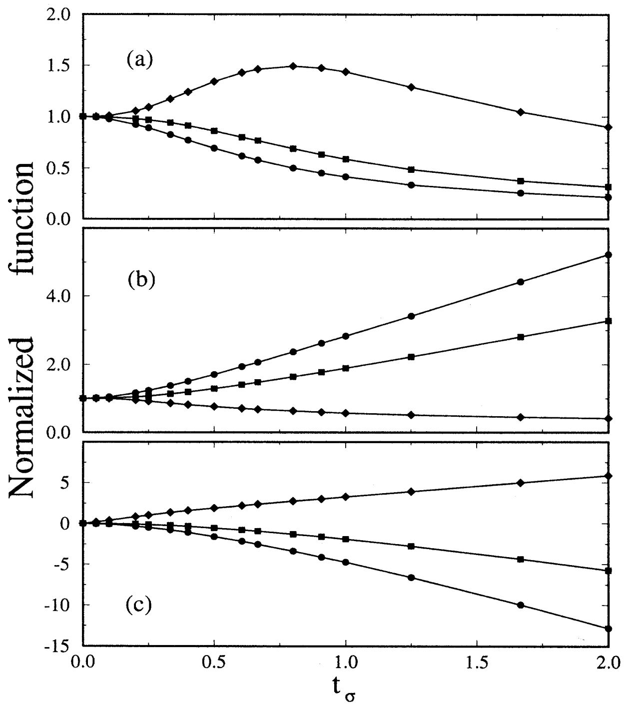

FIG. 1. Plot of the normalized energy and its first and second derivatives as a function of t_σ. (a) For exchange energy, $\widehat{E}_{x\sigma}(n_\sigma,t_\sigma)$ (circle), $\widehat{V}_{x\sigma}(n_\sigma,t_\sigma)$ (square), and $\widehat{K}_{x\sigma}(n_\sigma,t_\sigma)$ (diamond) are shown for α=0.5 (r_s=3.01). (b) For the kinetic part: plot of $\widehat{U}_{0\sigma}(n_\sigma,t_\sigma)$ (circle), $\widehat{V}_{0\sigma}(n_\sigma,t_\sigma)$ (square), and $\widehat{K}_{0\sigma}(n_\sigma,t_\sigma)$ (diamond). The two functions marked by circle and square in (b) increase, and $\widehat{K}_{0\sigma}$ decreases from their zero-temperature values at increasing t_σ. (c) For the entropy part: plot of $\widehat{S}_{s\sigma}(n_\sigma,t_\sigma)$ (circle), $\widehat{V}_{s\sigma}(n_\sigma,t_\sigma)$ (square), and $\widehat{K}_{s\sigma}(n_\sigma,t_\sigma)$ (diamond). The two functions marked by circle and square in (c) decrease, and $\widehat{K}_{s\sigma}$ increases from their zero-temperature values at increasing t_σ. Note that the normalized functions for the kinetic and entropy parts are independent of α. It is worth noting that the normalized functions of the noninteracting free energy part, especially those of the entropy part become dominant as temperature increases.

To investigate some properties in the next section, we need to consider the noninteracting thermodynamic potential $\Omega_0(n,s,T)$:

$$\Omega_0(n,s,T) \equiv \sum_\sigma \Omega_{0\sigma}(n_\sigma,T), \tag{41}$$

$$\Omega_{0\sigma}(n_\sigma,T) = \mathcal{U}_{0\sigma}(n_\sigma,T) - \mu_\sigma N_\sigma - TS_{0\sigma}(n_\sigma,T), \tag{42}$$

where $\mathcal{U}_{0\sigma} = \sum_{\mathbf p} \varepsilon_{\mathbf p} n_{\mathbf p\sigma}$ is the internal energy which is the kinetic energy for the noninteracting system, and $S_{0\sigma}$ is the entropy,

$$S_{0\sigma} = -k_B \sum_{\mathbf p}[n_{\mathbf p\sigma}\ln n_{\mathbf p\sigma} + (1-n_{\mathbf p\sigma})\ln(1-n_{\mathbf p\sigma})]. \tag{43}$$

Note that μ_σ in Eq. (42) is the chemical potential given in Eq. (14), not that of the noninteracting case. See Appendix A for discussions on the chemical potential.

First consider the internal energy per volume $U_0(n,s,T) \equiv \mathcal{U}_0(n,s,T)/\nu$. For each spin component we define the normalized quantity to its zero-temperature value $U_{0\sigma}(n_\sigma,0) = 3\mu^0_\sigma n_\sigma/5$,

$$\widehat{U}_{0\sigma}(n_\sigma,t_\sigma) = \frac{U_{0\sigma}(n_\sigma,T)}{U_{0\sigma}(n_\sigma,0)} = 5\int_0^\infty f_\sigma(x)x^4dx, \tag{44}$$

$$f_\sigma(x) = \frac{1}{e^{\xi_\sigma(x^2-1)-a^0_\sigma}+1}, \tag{45}$$

$$a^0_\sigma = \xi_\sigma \delta\mu^0_\sigma/\mu^0_\sigma, \tag{46}$$

where $\delta\mu^0_\sigma$ is the nonzero-temperature deviation in the chemical potential for the noninteracting system, and is determined by the similar condition to (29),

$$\int_0^\infty x^2dxf_\sigma(x) = \frac{1}{3}. \tag{47}$$

Similarly, we consider $V_{0\sigma}(n_\sigma,T)$ and $K_{0\sigma}(n_\sigma,T)$, which are the first and second derivatives of $U_{0\sigma}(n_\sigma,T)$ with respect to density, and define the normalized quantities $\widehat{V}_{0\sigma}(n_\sigma,t_\sigma)$ and $\widehat{K}_{0\sigma}(n_\sigma,t_\sigma)$ of $V_{0\sigma}(n_\sigma,T)$ and $K_{0\sigma}(n_\sigma,T)$ to $V_{0\sigma}(n_\sigma,0) = \mu^0_\sigma$ and $K_{0\sigma}(n_\sigma,0) = 2\mu^0_\sigma/3n_\sigma$, respectively:

$$\widehat{V}_{0\sigma}(n_\sigma,t_\sigma) = \widehat{U}_{0\sigma} + \frac{2\xi_\sigma}{5}\frac{d\widehat{U}_{0\sigma}}{d\xi_\sigma}, \tag{48}$$

$$\widehat{K}_{0\sigma}(n_\sigma,t_\sigma) = \widehat{U}_{0\sigma} + \frac{9\xi_\sigma}{5}\frac{d\widehat{U}_{0\sigma}}{d\xi_\sigma} + \frac{2\xi_\sigma^2}{5}\frac{d^2\widehat{U}_{0\sigma}}{d\xi_\sigma^2}. \tag{49}$$

The normalized functions for the internal energy are shown in Fig. 1(b). The functions $\widehat{U}_{0\sigma}$ (circle) and $\widehat{V}_{0\sigma}$ (square) increase from their zero-temperature values, while $\widehat{K}_{0\sigma}$ (diamond) decreases, at increasing t_σ. They are about of range over 0–6 for given t_σ. Compared to Fig. 1(a), $\widehat{V}_{0\sigma}$ and $\widehat{K}_{0\sigma}$ are larger in magnitude than corresponding functions in the exchange part. Note that the ratio of the exchange part to the noninteracting part is about α. This ratio appears later in Eqs. (52), (53), (72), and (77).

If we set $\mathcal{S}_{s\sigma}(n_\sigma,T) = -TS_{0\sigma}/\nu$, all formulas for the entropy part are the same as those for the internal energy with the replacement of $\widehat{U}_{0\sigma}(n_\sigma,t_\sigma)$ by $\widehat{\mathcal{S}}_{s\sigma}(n_\sigma,t_\sigma)$,

$$\widehat{\mathcal{S}}_{s\sigma}(n_\sigma,t_\sigma) = \frac{5}{\xi_\sigma}\int_0^\infty x^2dx\{f_\sigma(x)\ln f_\sigma(x) + [1-f_\sigma(x)]\ln[1-f_\sigma(x)]\}. \quad (50)$$

That is, $\widehat{V}_{s\sigma}$, $\widehat{K}_{s\sigma}$ are obtained by substitution of $\widehat{U}_{0\sigma}$ in Eqs. (48), (49), with $\widehat{\mathcal{S}}_{s\sigma}$. Note that the entropy part is normalized to the same normalizing factors as in the internal part. The normalized functions for the entropy part are shown in Fig. 1(c). The functions $\widehat{\mathcal{S}}_{s\sigma}$ (circle) and $\widehat{V}_{s\sigma}$ (square) decrease from their zero-temperature values, while $\widehat{K}_{s\sigma}$ (diamond) increases at t_σ. They are about of range over -15 to 10 for given t_σ. Comparing the behaviors of (a), (b), and (c) in Fig. 1, we see that the normalized functions of the noninteracting free energy, especially those of the entropy part become dominant as temperature increases.

Note that all functions marked by "hat" [e.g., $\widehat{E}_{x\sigma}(n_\sigma,t_\sigma)$, $\widehat{U}_{0\sigma}(n_\sigma,t_\sigma)$, etc.] except those for the entropy part, become 1 at the zero-temperature limit, while the hat functions for the entropy part become zero at the same limit.

III. APPLICATIONS

A. Energies

Consider the energies and potentials in the spin-polarized case. Using the results of the previous section, we obtain the total free energy per volume $\mathcal{F}_\nu(n,s,T)$:

$$\mathcal{F}_\nu(n,s,T) = U_0(n,s,T) + \mathcal{S}_s(n,s,T) + E_x(n,s,T). \quad (51)$$

With $U_0(n,0) = 3\mu^0 n/5$, which is the internal energy for $\zeta = 0$ at $T = 0$, we obtain the normalized free energy,

$$\frac{\mathcal{F}_\nu(n,s,T)}{U_0(n,0)} = \frac{1}{2}\sum_\sigma\left[(1+\sigma\zeta)^{5/3}(\widehat{U}_{0\sigma}+\widehat{\mathcal{S}}_{s\sigma}) - \frac{5\alpha}{2}(1+\sigma\zeta)^{4/3}\widehat{E}_{x\sigma}\right], \quad (52)$$

which at zero temperature reduces to the well-known expression,

$$\frac{\mathcal{F}_\nu(n,s,0)}{U_0(n,0)} = \frac{1}{2}\sum_\sigma\left[(1+\sigma\zeta)^{5/3} - \frac{5\alpha}{2}(1+\sigma\zeta)^{4/3}\right]. \quad (53)$$

Note that $\widehat{\mathcal{S}}_{s\sigma}$ in Eq. (52) has a factor of $(1+\sigma\zeta)^{-2/3}$ through ξ_σ^{-1}, as shown in Eq. (50). For α=0.5 (r_s = 3.01), Fig. 2 shows the normalized free energy (solid line) [Eq. (52)], the internal energy plus entropy part (dotted line), and the exchange energy (dot-dashed line) at t=0.0 (no symbol), 0.25 (circle), 0.5 (square), and 1.0 (diamond), respectively. Due to the entropy part, the dotted lines are changed very much compared to the dot-dashed lines as temperature increases. For α=0.5, we see that for given temperatures the paramagnetic state ($\zeta = 0$) always has the lowest energy.

It is well known that the HF electron gas with unscreened Coulomb interactions exhibits a ferromagnetic ($\zeta = 1$) instability for $r_s \cong 5.45$ at zero temperature, originally discovered by Bloch[18] in 1929. Partial polarizations ($0 < \zeta < 1$) were states of maxima. In connection with this fact, Fig. 2 implies that if temperature increases, we need a larger value of r_s for ferromagnetic instability or partially polarized state. Actually, given r_s larger than $r_s \cong 5.45$, there is a temperature T_c above which the paramagnetic state has the lowest energy. Between $T = 0$ and T_c, there is a partially-polarized state or a ferromagnetic state, which is minimum in energy, given T. This ferromagnetic theory of the electron gas using our self-consistent formalism will be studied in detail elsewhere.[19]

It is crucial that one understand ferromagnetic instability and the associated spin-wave properties of the system in the nonzero T case.[29] Following the SDF formalism, the transverse spin susceptibility $\chi_{+-}(q,\omega)$ is given by[16]

$$\chi_{+-}(q,\omega) = \frac{\chi_{+-}^{(0)}(q,\omega)}{1-(2W_x/s)\chi_{+-}^{(0)}(q,\omega)}, \quad (54)$$

$$\chi_{+-}^{(0)}(q,\omega) = -\int\frac{d^3k}{(2\pi)^3}\frac{n_{\mathbf{p}+} - n_{\mathbf{p}+\mathbf{q}-}}{-\hbar\omega - \mathcal{E}_+(\mathbf{p}) + \mathcal{E}_-(\mathbf{p}+\mathbf{q})}, \quad (55)$$

with

$$\mathcal{E}_\sigma(\mathbf{k}) = \hbar^2k^2/2m + V_x + \sigma W_x. \quad (56)$$

Note that $G_{x\perp}^{(2)} = W_x/s$, and that the spin waves are given by

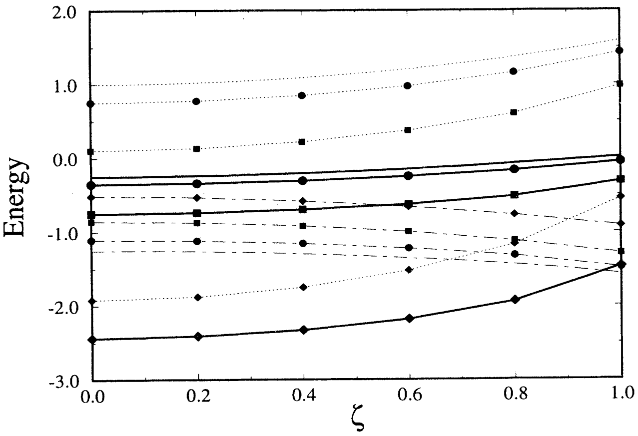

FIG. 2. Plot of the normalized free energy [Eq. (52)] of the spin-polarized electron gas as a function of ζ at t=0.0 (no symbol), 0.25 (circle), 0.5 (square), and 1.0 (diamond) for α=0.5 (r_s=3.01). The total free energy (solid line) consists of the internal energy, entropy part, and exchange energy. The internal energy plus the entropy part are represented by dotted lines, and the exchange energy, by dot-dashed lines. For example, the solid line with circles represent the normalized free energy at t=0.25.

$$2G^{(2)}_{x\perp}\chi^{(0)}_{+-}(q,\omega) = 1, \tag{57}$$

which has the property that for $q = 0$, $\omega = 0$. From Eq. (57), we obtain the spin-wave dispersion to be of the form

$$\hbar\omega_{\mathrm{SW}} = D_{\mathrm{LD}}(\zeta)(q/k_F)^2, \tag{58}$$

where

$$D_{\mathrm{LD}} = \frac{\hbar^2 k_F^2}{2m\zeta}\left[1 - \frac{1}{5\alpha}\frac{(1+\zeta)^{5/3}\widehat{U}_{0+} - (1-\zeta)^{5/3}\widehat{U}_{0-}}{(1+\zeta)^{1/3}\widehat{V}_{x+} - (1-\zeta)^{1/3}\widehat{V}_{x-}}\right]. \tag{59}$$

At zero temperature, this expression reduces to that of Rajagopal,[16] and Callaway and Wang,[20] who showed that the spin waves are stable for $5\alpha > 2^{4/3}$ (i.e., $r_s > 3.039$) for ferromagnetic ($\zeta = 1$) case.

This zero-temperature result should be compared with previous results by Rajagopal: For the ferromagnetic (ζ=1) state, spin waves are stable (i) for $r_s > 5.3447$,[12,21] and (ii) for $r_s > 5.4699$.[21] The first case was obtained by taking three terms in a series solution for the vertex function related to the transverse spin susceptibility. Taking four and five terms gives $r_s > 5.4106$ and $r_s > 5.4416$, respectively, for the stability of the spin wave.[21] The second one was obtained by solving the same vertex equation by a variational method. The second result is compatible with Herring's result,[22] which is $\hbar\omega_{\mathrm{SW}} \sim (\hbar^2q^2/2m)(1 - 5.485/r_s)$, in the sense that both results give the instability of the spin wave for the HF electron gas at $r_s \cong 5.45$, which was considered hints of the spin-density wave[23] state in the HFA.[21] In the viewpoint of previous results,[12,21–23] the present result (59) seems to be rather questionable even at $T = 0$, even though it was obtained by following a quite exact SDF theory.[16]

On the other hand, if we assume Eq. (59) to be correct, we can obtain D_{LD} for $T \neq 0$ by evaluating $\widehat{U}_{0\sigma}$ and $\widehat{V}_{x\sigma}$. For values the same as or close to $\zeta = 1$, we may expect that since $\widehat{U}_{0+}$ is larger than $\widehat{V}_{x+}$ for given $T \neq 0$ [see Figs. 1 (a),(b)], the spin waves become stable for values larger than $r_s = 3.039 + \delta$, being $\delta > 0$. This argument is valid as long as states close to $\zeta = 1$ have the lowest energy. This is related to the fact that as temperature increases r_s should be larger than 5.45 to obtain the ferromagnetic instability.

B. Potentials

In the local-spin-density approximation, the potentials are defined by

$$v^{\mathrm{xc}}_\sigma = \frac{\partial[n(\mathbf{r})\varepsilon^{\mathrm{xc}}(n(\mathbf{r}),\zeta(\mathbf{r}))]}{\partial n_\sigma(\mathbf{r})} \equiv \widetilde{\mu}^{\mathrm{xc}}_\sigma, \tag{60}$$

where $\varepsilon^{\mathrm{xc}}$ is the exchange-correlation energy per particle of the homogeneous spin-polarized electron gas and $\widetilde{\mu}^{\mathrm{xc}}_\sigma$ is its corresponding contribution to the chemical potential. The expression (60) is the generalization of that for the paramagnetic case: $v^{\mathrm{xc}} = \frac{\partial[n(\mathbf{r})\varepsilon^{\mathrm{xc}}(n(\mathbf{r}))]}{\partial n(\mathbf{r})} \equiv \widetilde{\mu}^{\mathrm{xc}}$.

Considering exchange effects only and noting the relation $n\varepsilon^x(n,\zeta) = E_x(n,s,T) = \sum_\sigma E_{x\sigma}(n_\sigma,T)$, we obtain

$$\frac{\partial[n\varepsilon^x(n,\zeta)]}{\partial n_\sigma} = \frac{dE_{x\sigma}(n_\sigma,T)}{dn_\sigma} = V_{x\sigma}(n_\sigma,T) \equiv \widetilde{\mu}^x_\sigma(T). \tag{61}$$

Similarly, we define for the noninteracting case

$$\frac{\partial[nu^0(n,\zeta)]}{\partial n_\sigma} = \frac{dU_{0\sigma}(n_\sigma,T)}{dn_\sigma} = V_{0\sigma}(n_\sigma,T), \tag{62}$$

$$\frac{\partial[nu^s(n,\zeta)]}{\partial n_\sigma} = \frac{dS_{s\sigma}(n_\sigma,T)}{dn_\sigma} = V_{s\sigma}(n_\sigma,T), \tag{63}$$

where u^0 and u^s are the internal energy and entropy per particle of the spin-polarized electron gas, respectively, and let $\widetilde{\mu}^0_\sigma(T)$ be their contribution to the chemical potential:

$$\widetilde{\mu}^0_\sigma(T) \equiv V_{0\sigma}(n_\sigma,T) + V_{s\sigma}(n_\sigma,T). \tag{64}$$

Two equations (61) and (64) are saying nothing but the Seitz theorem.[1] The Seitz theorem says that

$$\mu = \frac{d(nE_N)}{dn}, \tag{65}$$

where E_N is the ground-state energy per particle at zero temperature and is generalized to the free energy per particle $\mathcal{F}_N = \mathcal{F}_\nu/n$ at nonzero temperatures.

We check the Seitz theorem to see if our formalism meets self-consistency. Since generalization to the spin-polarized case is straightforward, consider the paramagnetic case without loss of generality. For the noninteracting electron gas at nonzero temperatures, we can determine the chemical potential $\mu_0(T) = \mu^0 + \delta\mu^0$, by considering the paramagnetic version of Eq. (47): $\int_0^\infty f(x)x^2dx = 1/3$, where $f(x)$ is the paramagnetic noninteracting occupation number. Here, μ^0 is the Fermi energy and $\delta\mu^0$ is its nonzero-temperature deviation. By the Seitz theorem, $\mu_0(T)$ should be the same as $\widetilde{\mu}^0(T) \equiv V_0(n,T) + V_s(n,T)$, where V_0, V_s are obtained by differentiating the paramagnetic internal energy and entropy part per volume with respect to density, respectively. Normalizing both sides of $\mu_0(T) = \widetilde{\mu}^0(T)$ by μ^0, we obtain

$$1 + a^0/\xi = \widehat{V}_0(n,t) + \widehat{V}_s(n,t), \tag{66}$$

where $a^0 = \xi\delta\mu^0/\mu^0$, and $\widehat{V}_0$ and $\widehat{V}_s$ are normalized quantities corresponding to V_0 and V_s, respectively.

This result is rather trivial and shown in Fig. 3(a). For the interacting electron gas with exchange effects, we can also determine the chemical potential $\mu(T) = \mu_0(T) + \mu_x(T)$, with $\eta = 1$, through the number conservation: $n = 2\sum_{\mathbf{p}} F(\eta{=}1,p)/\nu$, i.e.,

$$\int_0^\infty x^2dxF(\eta{=}1,x) = \frac{1}{3}. \tag{67}$$

Note that η should be 1 because the Seitz theorem relates

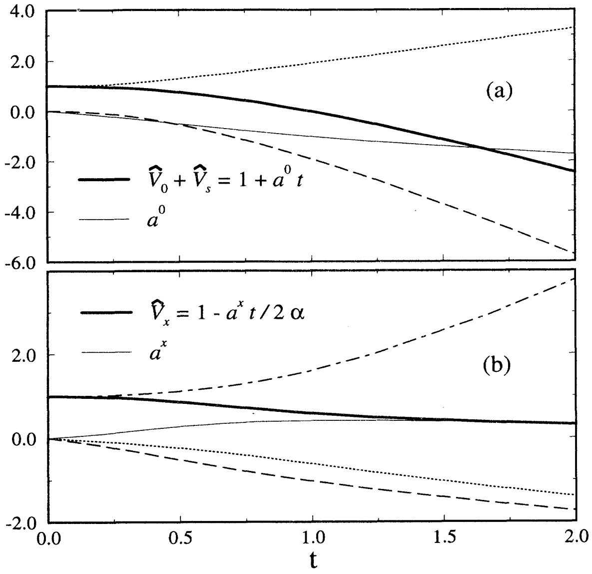

FIG. 3. Plot of testifying the Seitz theorem for the paramagnetic case. All the quantities are shown as a function of $t = 1/\xi$. (a) For the noninteracting case, $\hat V_0 + \hat V_s$ and $1 + a^0/\xi$ are shown to be exactly the same (bold solid line). For comparison, a^0 (light solid line), $\hat V_0$ (dotted), and $\hat V_s$ (dashed) are also shown. (b) For the interacting case with exchange effects, $\hat V_x$ and $1 - a^x/2\alpha\xi$ are also exactly the same (bold solid line) for α=0.5 (r_s=3.01). Here a^x (light solid line), a (dotted), a^0 (dashed), and $1 - a/2\alpha\xi$ (dot-dashed) are also given for comparison.

the chemical potential μ for the fully interacting ($\eta = 1$) electron gas and the total free energy $\mathcal{F}_\nu$.

From our calculations, we just determine $a = \xi\delta\mu/\mu^0$, where $\delta\mu$ is the total nonzero-temperature deviation in the chemical potential. Consider the decompositions $\mu_x(T) = \mu^x + \delta\mu^x$, where $\mu^x = -e^2 k_F/\pi$, and $\delta\mu = \delta\mu^0 + \delta\mu^x$. Thus, we obtain for $\delta\mu^x$,

$$\delta\mu^x = \delta\mu - \delta\mu^0, \qquad \text{i.e.,} \qquad a^x = a - a^0, \tag{68}$$

where $a^x = \xi\delta\mu^x/\mu^0$. Again, by the Seitz theorem, the relation

$$1 - \frac{a^x}{2\alpha\xi} = \hat V_x(n,t) \tag{69}$$

should be satisfied, where $\hat V_x$ is obtained by normalizing $V_x(n,T)$ by $V_x(n,0) = \mu^x$. $V_x(n,T)$ is the first derivative of the HF exchange energy $E_x(n,T)$ with respect to n in the paramagnetic case. It is worthwhile to note that the left-hand sides of Eqs. (66) and (69) come from the number conservation, and the right-hand sides of them, from the Seitz theorem. For more discussions on the chemical potential and the Seitz theorem, see Appendix A. For illustration, the results for α=0.5 (r_s=3.01) are shown in Fig. 3(b). Equation (69) is of course satisfied for other values of α.

The normalized potentials $\hat\mu^x_\sigma(T)$ for the exchange energy are obtained from $V_{x\sigma}(n_\sigma,T)$,

$$\hat\mu^x_\sigma(T) \equiv \frac{V_{x\sigma}(n_\sigma,T)}{V_x(n,0)} = (1+\sigma\zeta)^{1/3}\hat V_{x\sigma}(n_\sigma,t_\sigma), \tag{70}$$

where $\hat V_{x\sigma}(n_\sigma,t_\sigma)$ is obtained by Eq. (37). Note that $\hat V_{x\sigma}(n_\sigma,t_\sigma)$ can be also obtained by the spin-polarized version of Eq. (69): $1 - a^x_\sigma/2\alpha_\sigma\xi_\sigma = \hat V_{x\sigma}(n_\sigma,t_\sigma)$, where $a^x_\sigma = a_\sigma - a^0_\sigma$, with a_σ in Eq. (26) and a^0_σ in Eq. (46). Similarly, the potentials $\hat\mu^0_\sigma(T)$ for the noninteracting part are obtained from Eq. (64),

$$\begin{aligned}\hat\mu^0_\sigma(T) &\equiv \frac{V_{0\sigma}(n_\sigma,T) + V_{s\sigma}(n_\sigma,T)}{V_0(n,0)}\\ &= (1+\sigma\zeta)^{2/3}[\hat V_{0\sigma}(n_\sigma,t_\sigma) + \hat V_{s\sigma}(n_\sigma,t_\sigma)],\end{aligned} \tag{71}$$

where $V_0(n,0) = \mu^0$ is the Fermi energy. Similarly to Eq. (66), it is also satisfied that $1 + a^0_\sigma/\xi_\sigma = \hat V_{0\sigma}(n_\sigma,t_\sigma) + \hat V_{s\sigma}(n_\sigma,t_\sigma)$.

Figure 4 shows the potentials (a) $\hat\mu^x_\sigma(T)$ for α=0.5 (r_s=3.01), and (b) $\hat\mu^0_\sigma(T)$. In both Figs. 4(a) and (b), the solid and dashed lines represent spin-up and spin-down components, respectively, for t=0 (no symbol), t=0.25 (circle), t=0.5 (square), and t=1.0 (diamond). Due to temperature effects, the potentials become smaller as temperature increases. The potentials $\hat\mu^x_\sigma(T)$ are always positive. However, at nonzero temperatures, $\hat\mu^0_-(T)$ becomes negative as ζ increases and goes to $-\infty$ as $\zeta \to 1$.

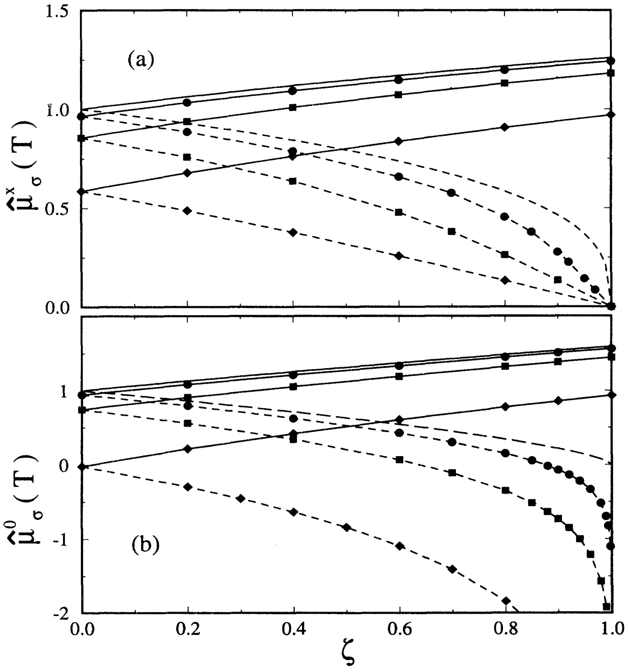

FIG. 4. (a) The exchange potentials $\hat\mu^x_\sigma(T)$ for α=0.5 (r_s=3.01), and (b) the potentials $\hat\mu^0_\sigma(T)$ of the noniteracting part as a function of ζ are shown at t=0.0 (no symbol), 0.25 (circle), 0.5 (square), and 1.0 (diamond). In both (a) and (b), solid lines represent spin-up components and dashed lines, spin-down components. The behaviors of $\hat\mu^x_+$ and $\hat\mu^0_+$ are similar, but note the difference between $\hat\mu^x_-$ and $\hat\mu^0_-$; at nonzero temperatures, $\hat\mu^0_-$ goes to $-\infty$ as $\zeta \to 1$, while $\hat\mu^x_-$ is 0 at $\zeta = 1$.

[In fact, the quantity $\widehat{V}_{s\sigma}(n_\sigma, t_\sigma)$ becomes $-\infty$ as $\zeta \to 1$.] Compare this behavior with that of $\widehat{\mu}^x_-(T)$, which is 0 at $\zeta = 1$.

This singular behavior in $\widehat{\mu}^0_-(T)$ is related to the fact that the fraction of spin-down component n_- reduces to zero as $\zeta \to 1$: That is, in the noninteracting Fermi-Dirac function f_σ [Eq. (45)], the effective temperature $t_\sigma = \xi_\sigma^{-1}$ becomes very large and thus the chemical potential μ^0_σ becomes negative and very much smaller than $-k_BT$, which corresponds to the classical limit; the Fermi-Dirac function f_σ reduces to the usual Maxwell-Boltzmann expression.

If we define the normalized total potentials as $\widehat{\mu}_\sigma(T) = [\widetilde{\mu}^0_\sigma(T) + \widetilde{\mu}^x_\sigma(T)]/\mu^0$, we obtain

$$\widehat{\mu}_\sigma(T) = \widehat{\mu}^0_\sigma(T) - 2\alpha\widehat{\mu}^x_\sigma(T). \tag{72}$$

From Fig. 4, we can deduce that for the spin-down component $\widehat{\mu}_-(T)$, effects of the noninteracting part are manifest as temperature increases, especially at large ζ.

C. Compressibility

The pressure P is defined as the rate of change in E with volume at constant N. The inverse compressibility is the rate of change of P under the same conditions:[1]

$$P = -\left(\frac{dE}{d\nu}\right)_N, \tag{73}$$

$$\frac{1}{K} = -\nu\left(\frac{dP}{d\nu}\right)_N = n^2\frac{d^2(E/\nu)}{dn^2}, \tag{74}$$

where E is the total ground-state energy of the system at zero temperature. At nonzero temperatures, this is generalized to represent the total free energy $\mathcal{F} = \nu\mathcal{F}_\nu$, where $\mathcal{F} = \mathcal{F}_+ + \mathcal{F}_-$. Then, the inverse compressibility at constant magnetization $M = N\zeta$ can be expressed as

$$\frac{1}{K_M} = n^2\frac{d^2(\mathcal{F}_\nu)}{dn^2} = \sum_\sigma n_\sigma^2\frac{d^2(\mathcal{F}_{\nu\sigma})}{dn_\sigma^2}, \tag{75}$$

from which we obtain

$$\frac{1}{K_M} = \sum_\sigma n_\sigma^2(K_{0\sigma} + K_{s\sigma} + K_{x\sigma}), \tag{76}$$

$$\frac{K_F}{K_M} = \frac{1}{2}\sum_\sigma[(1+\sigma\zeta)^{5/3}(\widehat{K}_{0\sigma} + \widehat{K}_{s\sigma}) -\alpha(1+\sigma\zeta)^{4/3}\widehat{K}_{x\sigma}], \tag{77}$$

where $K_F = 3/(2\mu^0 n)$ is the compressibility of the noninteracting gas at zero temperature.

The results for the compressibility are shown in Fig. 5 at t=0.0 (no symbol), 0.25 (circle), 0.5 (square), and 1.0 (diamond) for α=0.5 (r_s=3.01). Solid lines represent contributions from the total free energy, and dotted lines, those from the noninteracting part, while dashed lines represent exchange effects. Due to entropy effects as in Fig. 2, the compressibility from the noninteracting free energy is changed very much as temperature increases, while contributions from the exchange energy are not changed much.

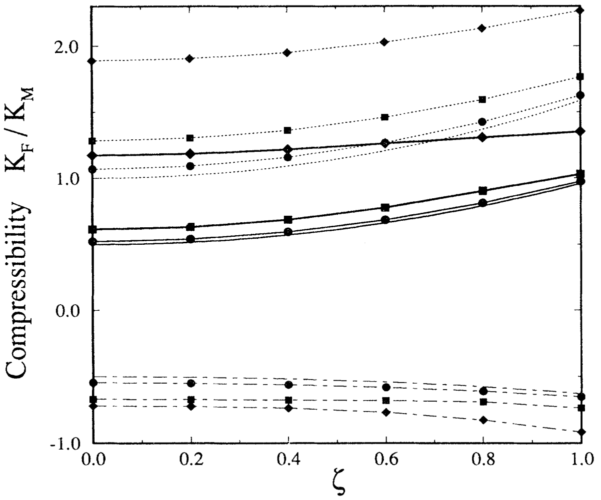

FIG. 5. The compressibility at constant magnetization at t=0.0 (no symbol), 0.25 (circle), 0.5 (square), and 1.0 (diamond) for α=0.5 (r_s=3.01). Solid lines represent contributions from the total free energy, and dotted lines, those from the noninteracting free energy, while dot-dashed lines represent only exchange effects. Note that contributions from the exchange energy are similar in magnitude for three t values, but those from the noninteracting part show big differences due to entropy effects.

D. Polarization

Consider the polarization $P(q)$, which consists of two contributions from each spin:

$$P(q) = P_+(q) + P_-(q). \tag{78}$$

In the long-wavelength limit, the compressibility sum rule[1,24] says

$$P(0) = -\frac{\partial n}{\partial\mu}, \tag{79}$$

$$P_\sigma(0) = -\frac{\partial n_\sigma}{\partial\mu_\sigma}. \tag{80}$$

Within the HFA, differentiating Eq. (14) for μ_σ, with respect to $n_\sigma = k_\sigma^3/6\pi^2$, we obtain

$$P_{x\sigma}(0) = \frac{-\rho_{0\sigma}}{1 - \alpha_\sigma + \partial_{\xi_\sigma}a_\sigma}, \tag{81}$$

$$\rho_{0\sigma} = \frac{3n_\sigma}{2\mu^0_\sigma} = \frac{1}{2}\rho_0(1+\sigma\zeta)^{1/3}, \tag{82}$$

and thus

$$P_x(0) = -\frac{1}{2}\rho_0\sum_\sigma\frac{(1+\sigma\zeta)^{1/3}}{1 - \alpha_\sigma + \partial_{\xi_\sigma}a_\sigma}, \tag{83}$$

where $\rho_{0\sigma}$ is the noninteracting density of states for spin σ, corresponding to $\rho_0 = 3n/2\mu^0$ and $\partial_{\xi_\sigma} a_\sigma$ is the nonzero-temperature contribution, which for given ζ is determined by the derivative, with respect to ξ_σ, of the number conservation (29) when η=1:

$$\int_0^\infty x^2 dx \partial_{\xi_\sigma} F_\sigma(\eta{=}1, x) = 0. \tag{84}$$

For the noninteracting case, the second term in the denominator of Eq. (83) vanishes and the third one becomes $\partial_{\xi_\sigma} a_\sigma^0$, because there is no exchange effect. For the paramagnetic case, Eq. (83) reduces to

$$P_x(0) = -\frac{\rho_0}{1 - \alpha + \partial_\xi a} \equiv -r_s \rho_0 \widetilde{P}_x(0), \tag{85}$$

where $\partial_\xi a$ is determined by the derivative of Eq. (67) with respect to ξ.

For comparison, we consider the following formulas:[11]

$$P(q) = (1 + C)^{-1} \overline{P}^0(q), \tag{86}$$

$$\overline{P}^0(q) = (P_+^0, P_-^0), \tag{87}$$

$$C_{\sigma,\sigma'} = -P_\sigma^0 \frac{\partial \widetilde{\mu}_\sigma^{\mathrm{xc}}}{\partial n_\sigma}, \tag{88}$$

where P_σ^0 is the polarization for spin σ for the random-phase approximation. If only exchange effects are considered, the matrix C becomes diagonal because only electrons with the same spin can be exchanged. Noting the relation $K_{x\sigma}(n_\sigma, T) = \frac{\partial \widetilde{\mu}_\sigma^x}{\partial n_\sigma}$, we obtain

$$P_x(q) = \sum_\sigma \frac{P_\sigma^0(q)}{1 - P_\sigma^0(q) K_{x\sigma}(n_\sigma, T)}, \tag{89}$$

which becomes in the long-wavelength limit for the paramagnetic case

$$P_x(0) = \frac{P^0}{1 - P^0 K_x(n, T)}. \tag{90}$$

Using the relations $\widehat{K}_{x\sigma} \doteq K_{x\sigma}(n_\sigma, T)/K_{x\sigma}(n_\sigma, 0)$ and $P_\sigma^0(0) = -\rho_{0\sigma} h_\sigma(t_\sigma)$, where $h_\sigma(t_\sigma) = \int_0^\infty dx f_\sigma(x)$, the above formula (89) in the long-wavelength limit reduces to

$$P_x(0) = -\frac{1}{2}\rho_0 \sum_\sigma \frac{(1 + \sigma\zeta)^{1/3} h_\sigma(t_\sigma)}{1 - \alpha h_\sigma(t_\sigma) \widehat{K}_{x\sigma}/(1 + \sigma\zeta)^{1/3}}. \tag{91}$$

On the other hand, we consider the polarization within conserving approximations.[25–28] The spin-polarized case is a straightforward generalization of the paramagnetic one in Ref. 25. Thus, we obtain

$$P_x(0) = -\sum_\sigma \gamma_\sigma \rho_{0\sigma}, \tag{92}$$

$$\gamma_\sigma = \xi_\sigma \int_0^\infty \frac{y^2 dy \Gamma_\sigma(y)}{1 + \cosh G_\sigma(y)}, \tag{93}$$

$$\Gamma_\sigma(x) = 1 + \frac{\alpha_\sigma \xi_\sigma}{x} \int_0^\infty \frac{y dy \Gamma_\sigma(y)}{1 + \cosh G_\sigma(y)} \ln\left|\frac{x + y}{x - y}\right|, \tag{94}$$

where $G_\sigma(y)$ is simply obtained by setting $\eta = 1$ in Eqs. (23)–(28). It is worthwhile to note works of Rajagopal *et al.*,[12] where derivations of all relevant response functions expressed in terms of appropriate vertex functions and the associated integral equations for the vertex functions were given. A careful comparison shows that our formalism in conserving approximations can also be obtained by considering a special case of their formalism, i.e., the Hartree-Fock case with unscreened potential.

If a screening parameter $\lambda(q)$ is defined by $\epsilon(q) = 1 + \lambda^2(q)/q^2$, i.e., $\lambda^2(q) = -4\pi e^2 P(q)$, there is a relation[11] between $\lambda(0)$ and K_B, the compressibility at constant magnetic field B,

$$[\lambda(0)/q_{\mathrm{TF}}]^2 = K_B/K_F, \tag{95}$$

where q_{TF} is the Thomas-Fermi wave vector and K_F is defined earlier. Thus, if we calculate the polarization, the

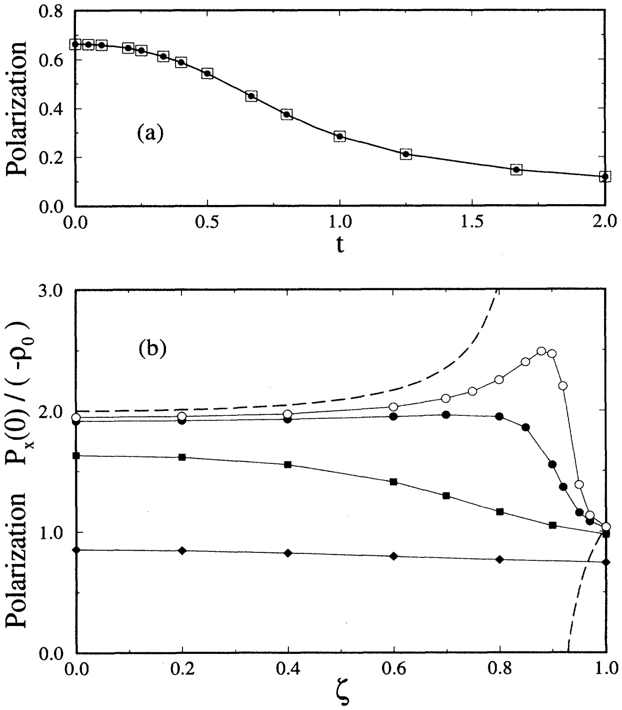

FIG. 6. Plot of polarizations for (a) the paramagnetic case and (b) the spin-polarized one. (a) Normalized polarizations $P_x(0)/(-r_s\rho_0)$ as a function of t for the paramagnetic case for α=0.5 (r_s=3.01). Three results are exactly the same. The solid lines are the results of $\widetilde{P}_x(0)$ in Eq. (85), while the filled circles and open squares are the same as $\widehat{\chi}_P(n, t)$ and $\widehat{P}_x(0)$ in Refs. 7 and 25, respectively. (b) Polarizations $P_x(0)/(-\rho_0)$ for the spin-polarized system for α=0.5. The dashed lines are for t=0.0 (no symbol), which show a divergence around $\zeta \sim 0.87$. The open and filled circles correspond to t=0.2 and 0.25, respectively. Squares and diamonds represent results for t=0.5 and 1.0. The polarizations are obtained by three methods explained in text. These three results are of course the same as in the paramagnetic case. For simplicity, they are represented as one symbol. The results for nonzero temperatures do not show any divergence, which means that there is a point, between t=0.0 and 0.2, above which the negative screening disappears.

compressibility K_B can be automatically obtained using Eq. (95).

Figure 6 shows results for (a) the paramagnetic and (b) spin-polarized cases. For α=0.5 (r_s = 3.01), the polarization $\widetilde{P}_x(0)$ in Eq. (85) is shown as a solid line in Fig. 6(a), where two other results (filled circle and open square with no line) from the previous works[7,25] are also shown for comparison. Three results are exactly the same. The filled circles are nothing but Eq. (90), which is the same as the long-wavelength limit of the formula $\chi_p(n,t)/(-g^2\mu_B^2) = \chi_0/[1-K_x(n,T)\chi_0]$ used in Ref. 7. There, we evaluated normalized quantity $\widehat{\chi}_p(n,t)$, which is shown here as filled circles. Open squares are the results obtained for the paramagnetic case by conserving approximations, where the vertex functions are solved self-consistently by iterations and used to obtain the polarization.[25] The results (open square and filled circle) by the latter two methods have been already shown in Fig. 3 of Ref. 25, where the polarizations for other α values (α=0.1, 0.3, 0.7, 0.8 and 0.9) were also calculated. Since for the paramagnetic case, polarizations obtained by three methods are exactly the same [see Fig. 6 (a)], this sameness is also expected for the spin-polarized case.

Now consider polarizations for the spin-polarized system, which are shown in Fig. 6(b). The dashed lines represent zero-temperature result, and the nonzero-temperature results for α=0.5 (r_s=3.01) are shown at t=0.2 (open circle), t=0.25 (filled circle), 0.5 (square), and 1.0 (diamond). They were evaluated by three different methods; (i) using Eq. (83), (ii) using Eq. (91), and (iii) from conserving approximations [Eqs. (92)−(94)]. These three methods yield the same results as in the paramagnetic case, which are represented as one symbol.

In Fig. 6(b), note a divergence and negative polarizations over a region of $\zeta \sim 0.87$ at zero temperature, which would give a negative screening.[30,31] However, this negative screening would be considered unphysical, because when correlation effects are considered there is no sign of negative screening.[11,32] On the other hand, the results for nonzero temperatures may indicate that as temperature increases the negative screening seems to disappear, and that there is a temperature point, between t=0 and 0.2, above which the negative screening disappear. The negative polarization region is replaced by a peak at increasing t, and finally the peak smooths out.

IV. SUMMARY AND DISCUSSION

In the previous paper[7] and this paper, we have been dealing with a homogeneous electron gas, by performing a coupling-constant integral with the correct Fermi-Dirac functions. Especially in this paper, the spin-polarized electron gas has been investigated, considering spin summations explicitly. The exchange-only scheme has been used to calculate the free energy, which consists of the HF exchange energy and the internal energy and entropy part. Their functional derivatives with respect to density are also calculated at nonzero temperatures. Since Coulomb interactions are spin independent and so the exchange self-energy is decoupled into up- and down-spin components, the quantities considered are totally decoupled for spin. Thus, generalization of the previous formalism for the paramagnetic system to spin-polarized one was straightforward.

At zero temperature, the correct Fermi-Dirac function reduces to the noninteracting Fermi-Dirac function, because of normalization of the chemical potential. The difference between our exchange-only scheme and the lowest-order HFA becomes manifest at nonzero temperatures. In the viewpoint of the coupling-constant-integral formalism with the correct Fermi-Dirac function, our exchange-only scheme is indeed a self-consistent generalization of the usual HFA at nonzero temperatures.

Using our self-consistent formalism, we calculated some properties such as the total free energy, potentials, compressibility, and polarization. These properties have been already considered at zero temperature by Gunnarsson and Lundqvist.[11] Here, we focused on nonzero-temperature behaviors. As temperature increases, the noninteracting free energy decreases faster than the rate at which the exchange energy increases, so the total free energy decreases. The normalized potentials become smaller as temperature increases. The spin-down components of the noninteracting potentials become negative, due to the entropy part at nonzero temperatures. The total compressibility at constant magnetization increases at temperature, due to the fast increase of the compressibility of the noninteracting electron gas. The polarization decreases at increasing temperature, and here it is worth noting the disappearance of the negative screening at nonzero temperatures.

Here, we wish to compare our formalism with others in the viewpoint of the kinetic contribution to the exchange-correlation energy, $T_{\rm xc}[n]$, which has been studied only at zero temperature by many authors,[33–36] as far as we know. $T_{\rm xc}[n]$ is defined by

$$T_{\rm xc}[n] \equiv \langle\Psi_{[n]}|\widehat{T}|\Psi_{[n]}\rangle - \langle\Psi^0_{[n]}|\widehat{T}|\Psi^0_{[n]}\rangle, \tag{96}$$

where $\Psi_{[n]}$ is the exact Hohenberg-Kohn[37] interacting ground-state wave function and $\Psi^0_{[n]}$, the corresponding Kohn-Sham[38] noninteracting wave function. The expression for $T_{\rm xc}$, known as the Bass's equation,[35] was obtained for zero temperature,

$$T_{\rm xc}[n] = a_B\frac{\partial\Omega_{\rm xc}[n]}{\partial a_B} = a_B\frac{\partial\Omega_c[n]}{\partial a_B}, \tag{97}$$

where the second equality comes from the fact that the exchange energy does not explicitly depend on a_B at zero temperature.

Now apply the above formula (97) for $T_{\rm xc}$ to our exchange-only scheme. Without loss of generality, consider the paramagnetic case. In Ref. 7, we have for the exchange energy per volume $E_x(n,T) = \Omega_x(n,T)/\nu$,

$$E_x(n,T) = E_x(n,0)\widehat{E}_x(a_B^3 n,t), \tag{98}$$

$$\begin{aligned} V_x(n,T) &= \frac{dE_x(n,T)}{dn} = V_x(n,0)\widehat{V}_x(a_B^3 n,t) \\ &= V_x(n,0)\left[\widehat{E}_x + \frac{\xi}{2}\frac{d\widehat{E}_x}{d\xi}\right], \end{aligned} \tag{99}$$

where $E_x(n,0){=}-e^2k_F^4/4\pi^3$ and we gave an explicit dependence on a_B to $\hat{E}_x$, which becomes 1 at zero temperature. Since at zero temperature our exchange energy $E_x(n,0)$ does not depend explicitly on a_B, the kinetic contribution to the exchange energy T_x becomes zero. However, at nonzero temperatures our $E_x(n,T)$ depends on a_B through $\hat{E}_x(a_B^3n,t)$, because of the exchange self-energy correction in the Fermi-Dirac function. Even if the second equality in Eq. (97) is incorrect at nonzero temperatures in our exchange-only scheme, the first one is still correct. For a simple generalization of Eq. (97) to the nonzero-temperature case, see Appendix B. With $\Omega_x[n] = \nu E_x(n,T)$ and $T_x = \nu\mathcal{T}_x$, we obtain

$$\begin{aligned}\mathcal{T}_x &= a_B\frac{\partial E_x(n,T)}{\partial a_B} = E_x(n,0)a_B\frac{\partial \hat{E}_x(a_B^3n,t)}{\partial a_B}\\ &= E_x(n,0)3n\frac{\partial \hat{E}_x(a_B^3n,t)}{\partial n} = E_x(n,0)2\xi\frac{d\hat{E}_x}{d\xi}\\ &= 4E_x(n,0)[\hat{V}_x(n,t) - \hat{E}_x(n,t)], \qquad (100)\end{aligned}$$

where we used $dn{=}\frac{3n}{2\xi}d\xi$ in the second line and $\hat{V}_x{-}\hat{E}_x{=}\frac{\xi}{2}\frac{d\hat{E}_x}{d\xi}$ in the last line. Note that Eq. (100) becomes zero at zero temperature, because both $\hat{E}_x$ and $\hat{V}_x$ become 1 at $T = 0$. The difference $\hat{V}_x(n,t) - \hat{E}_x(n,t)$ can be easily shown in Fig. 1 of Ref. 7. We thus obtain a nonzero contribution to T_x at nonzero temperatures, if our coupling-constant-integral formalism is adopted. This becomes manifest, since we consider all higher-order corrections in addition to lowest-order HF term by doing a coupling-constant integral and the higher-order terms have been usually included in the correction terms for correlation effects. The correlation effects we considered are effective only at nonzero temperatures, since they are just normalized into the chemical potential at zero temperature.

ACKNOWLEDGMENTS

We acknowledge research support from the University of Tennessee and from the U.S. Department of Energy through Contract No. DE-AC05-84OR21400 administered by Martin Marietta Energy Systems.

APPENDIX A: NOTE ON THE CHEMICAL POTENTIAL AND THE SEITZ THEOREM

Since the generalization to the spin-polarized case is straightforward, we consider the paramagnetic case. If we consider only exchange effects, the thermodynamic potential Ω can be written down by $\Omega = \Omega_0 + \Omega_x$. Since Ω_0 is the noninteracting thermodynamic potential, it is tempting to express it as

$$\Omega_0 = \mathcal{U}_0 - \mu_0 N - TS_0, \qquad (A1)$$

$$\mathcal{F}_0 = \mathcal{U}_0 - TS_0. \qquad (A2)$$

Noting that $\mu(T) = \mu_0(T) + \mu_x(T)$, we may guess that Ω_x would contain $\mu_x(T)$ and so would be decomposed into three pieces like Ω_0,

$$\Omega_x = \mathcal{U}_x - \mu_x N - TS_x \equiv \mathcal{F}_x - \mu_x N. \qquad (A3)$$

Consider the chemical potential using the Seitz theorem, Eq. (65). For the noninteracting case, we obtain

$$\mu_0(T=0) = \frac{d(\mathcal{U}_0/\nu)}{dn} = \mu^0 = \frac{\hbar^2k_F^2}{2m}, \qquad (A4)$$

$$\mu_0(T) = \frac{d(\mathcal{F}_0/\nu)}{dn}, \qquad (A5)$$

and if Eq. (A3) were correct, it would be also correct to obtain μ_x, using the relation

$$\mu_x(T) = \frac{d(\mathcal{F}_x/\nu)}{dn}. \qquad (A6)$$

However, this is not correct because we have already obtained $\mu_x(T)$ in Sec. III B through the formula

$$\mu_x(T) = \frac{d(\Omega_x/\nu)}{dn} = \frac{dE_x}{dn}, \qquad (A7)$$

which means that Ω_x do not have the term $-\mu_x N$, so one may wonder where μ_x is in the thermodynamic potential Ω.

It looks like a contradiction. How can it be resolved? The above argument was wrong because the wrong equation (A3) was used. Before correcting them, consider the definition of the chemical potential. For convenience, let us consider the grand canonical ensemble, which is the appropriate ensemble for use in a many-body theory. In this ensemble, all the thermodynamic properties can be deduced from the grand partition function Z_G, i.e., the thermodynamic potential Ω:[8]

$$Z_G = e^{-\beta\Omega} = \mathrm{Tr}[e^{-\beta(H-\mu\hat{N})}], \qquad (A8)$$

$$\Omega = \Omega_0 - \frac{1}{\beta}\sum_l U_l, \qquad (A9)$$

$$\begin{aligned}\Omega_0 = 2\sum_{\mathbf{p}}(\varepsilon_{\mathbf{p}} - \mu)n_{\mathbf{p}} + 2k_BT\sum_{\mathbf{p}\sigma}[n_{\mathbf{p}}\ln n_{\mathbf{p}}\\ +(1-n_{\mathbf{p}})\ln(1-n_{\mathbf{p}})], \qquad (A10)\end{aligned}$$

$$U_l = \frac{(-1)^l}{l}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_l\langle T_\tau V(\tau_1)\cdots V(\tau_l)\rangle, \qquad (A11)$$

where V is the electron-electron interaction. In the last expression, only different connected diagrams are evaluated, and in the exchange-only scheme, $\sum_l U_l$ becomes $-\beta\Omega_x$. The change of the thermodynamic potential Ω is

$$d\Omega = -Pd\nu - SdT - \overline{N}d\mu, \qquad (A12)$$

from which we deduce the average number $\overline{N}$:

$$\overline{N} = -\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,\nu}. \qquad (A13)$$

On the other hand, the grand partition function Z_G can be written in terms of the partition function Q_N:[39]

$$Z_G(T,\nu,\mu) = \sum_{N=0}^{\infty} e^{\beta\mu N} Q_N(T,\nu) \equiv \sum_{N=0}^{\infty} W(N), \tag{A14}$$

$$Q_N(T,\nu) = \mathrm{Tr}\ (e^{-\beta H}) = e^{-\beta\mathcal{F}(T,\nu,N)}, \tag{A15}$$

where $\mathcal{F}(T,\nu,N)$ is the (Helmholtz) free energy. When the density fluctuations are small, $W(N)$ is strongly peaked about $N = \overline{N}$, the average number, with a width of the order of $\sqrt{\overline{N}}$. Thus, we obtain

$$Z_G = e^{-\beta\Omega} \approx W(N=\overline{N}) = e^{\beta\mu\overline{N}} e^{-\beta\mathcal{F}}, \tag{A16}$$

that is, the free energy $\mathcal{F}(T,\nu,N)$ is directly obtained from the thermodynamic potential Ω through the formula

$$\mathcal{F}(T,\nu,N) = \Omega(T,\nu,\mu) + \mu N, \tag{A17}$$

where the bar on $\overline{N}$ was and will be below dropped out for convenience and μ is determined by Eq. (A13).

In the canonical ensemble (where N is fixed as in our system considered), one deals instead of Ω with the free energy $\mathcal{F}$,

$$\mathcal{F} = \Omega + \mu N, \tag{A18}$$

$$d\mathcal{F} = -Pd\nu - SdT + \mu dN, \tag{A19}$$

in terms of which the chemical potential is given by

$$\mu = \left(\frac{\partial\mathcal{F}}{\partial N}\right)_{T,\nu}. \tag{A20}$$

From the relation $\mathcal{F} \equiv N\mathcal{F}_N = \nu\mathcal{F}_\nu = \nu n\mathcal{F}_N$,

$$\begin{aligned}\mu &= \mathcal{F}_N + N\left(\frac{\partial\mathcal{F}_N}{\partial N}\right)_{T,\nu}\\ &= \mathcal{F}_N + n\frac{d\mathcal{F}_N}{dn} = \frac{d\mathcal{F}_\nu}{dn},\end{aligned} \tag{A21}$$

which is the Seitz theorem, Eq. (65).

Now consider Ω_0. To obtain Eq. (A1) from Eq. (A10), we considered $\xi_{\mathbf{p}}$ to be $\varepsilon_{\mathbf{p}} - \mu_0$. This is not correct. This should be $\varepsilon_{\mathbf{p}} - \mu$, where in the exchange-only scheme μ consists of μ_0 and the correction from the interactions μ_x. For the noninteracting case, the chemical potential was $\mu = \mu_0$ in Eq. (A10), but when the interaction is turned on, it should be changed to μ. Since the chemical potential is just a number, Ω_0 becomes for an interacting case

$$\Omega_0 = \mathcal{U}_0 - \mu N - TS_0 = \mathcal{F}_0 - (\mu_0 + \mu_x)N, \tag{A22}$$

where we used the relation $\mu = \mu_0 + \mu_x$. Note that $n_{\mathbf{p}}$ in Eq. (A10) remains as the noninteracting occupation number even when the interaction is on. That is, $\mu_x N$ is an additional term due to electron interactions, which should be extracted from the noninteracting thermodynamical potential and so Eq. (A9) should have been written down as

$$\Omega = \widetilde{\Omega}_0 - \mu_x N + \Omega_x \equiv \widetilde{\Omega}_0 + \widetilde{\Omega}_x, \tag{A23}$$

where $\widetilde{\Omega}_0$ is the purely noninteracting piece, Eq. (A10) with μ_0 instead of μ, and $\widetilde{\Omega}_x$ is the remaining. From the relation

$$\begin{aligned}\Omega &= \Omega_0 + \Omega_x = \mathcal{F} - \mu N\\ &= (\mathcal{F}_0 + \Omega_x) - (\mu_0 + \mu_x)N,\end{aligned} \tag{A24}$$

we can obtain μ through the formulas

$$\mu = \frac{d\mathcal{F}_\nu}{dn} = \frac{d(\mathcal{F}_0/\nu)}{dn} + \frac{d(\Omega_x/\nu)}{dn}, \tag{A25}$$

$$\mu_0 = \frac{d(\mathcal{F}_0/\nu)}{dn}, \tag{A26}$$

$$\mu_x = \frac{d(\Omega_x/\nu)}{dn}. \tag{A27}$$

Thus our contradictory case is resolved.

APPENDIX B: NOTE ON THE KINETIC PART OF THE EXCHANGE-CORRELATION ENERGY

Here, we wish to generalize the zero-temperature formula (97) to the nonzero-temperature case. We first summarize the work by Görling *et al.*,[33] which will be followed for the extension to the nonzero-temperature case. For comparison to be easier, we just use notations by Görling *et al.* They defined ${}^{\gamma}\Psi^{\alpha,\beta}_{[n]}$ as the wave function which minimizes $\langle\Psi|\alpha\widehat{T}+\beta\widehat{V}_{ee}+\gamma\widehat{A}|\Psi\rangle$, where $\widehat{T}$ and $\widehat{V}_{ee}$ are the operators for the kinetic and electron-electron repulsion energies, respectively, and $\widehat{A}$ is an arbitrary general quantum-mechanical operator. It follows then that ${}^{0}\Psi^{1,1}_{[n]}$ is the exact Hohenberg-Kohn[37] interacting ground-state wave function and ${}^{0}\Psi^{1,0}_{[n]}$, the corresponding Kohn-Sham[38] noninteracting wave function. They also defined the exchange and correlation energies with γ included,

$${}^{\gamma}E^{\alpha,\beta}_{x}[n] = \langle{}^{\gamma}\Psi^{\alpha,0}_{[n]}|\beta\widehat{V}_{ee}|{}^{\gamma}\Psi^{\alpha,0}_{[n]}\rangle - \beta U[n], \tag{B1}$$

$$\begin{aligned}{}^{\gamma}E^{\alpha,\beta}_{c}[n] &= \langle{}^{\gamma}\Psi^{\alpha,\beta}_{[n]}|\alpha\widehat{T}+\beta\widehat{V}_{ee}+\gamma\widehat{A}|{}^{\gamma}\Psi^{\alpha,\beta}_{[n]}\rangle\\ &\quad -\langle{}^{\gamma}\Psi^{\alpha,0}_{[n]}|\alpha\widehat{T}+\beta\widehat{V}_{ee}+\gamma\widehat{A}|{}^{\gamma}\Psi^{\alpha,0}_{[n]}\rangle,\end{aligned} \tag{B2}$$

with

$$U[n] = \frac{1}{2}\int\int d\mathbf{r}d\mathbf{r}'n(\mathbf{r})n(\mathbf{r}')|\mathbf{r}-\mathbf{r}'|^{-1}. \tag{B3}$$

Here, note that in their definition ${}^{\gamma}E^{\alpha,\beta}_{x}[n]$ with α=β=1, i.e., the usual HF exchange energy, is independent of γ. The total exchange-correlation energy ${}^{\gamma}E^{\alpha,\beta}_{\mathrm{xc}}[n] \equiv {}^{\gamma}E^{\alpha,\beta}_{x}[n] + {}^{\gamma}E^{\alpha,\beta}_{c}[n]$ is given by

$$\begin{aligned}{}^{\gamma}E^{\alpha,\beta}_{\mathrm{xc}}[n] &= \langle{}^{\gamma}\Psi^{\alpha,\beta}_{[n]}|\alpha\widehat{T}+\beta\widehat{V}_{ee}+\gamma\widehat{A}|{}^{\gamma}\Psi^{\alpha,\beta}_{[n]}\rangle\\ &\quad -\langle{}^{\gamma}\Psi^{\alpha,0}_{[n]}|\alpha\widehat{T}+\gamma\widehat{A}|{}^{\gamma}\Psi^{\alpha,0}_{[n]}\rangle - \beta U[n].\end{aligned} \tag{B4}$$

They obtained the generalized form of the Bauer relation[34]

$$\left.\frac{\partial}{\partial\gamma}{}^{\gamma}E^{\alpha,\beta}_{xc}[n]\right|_{\gamma=0} = \langle{}^{0}\Psi^{\alpha,\beta}_{[n]}|\widehat{A}|{}^{0}\Psi^{\alpha,\beta}_{[n]}\rangle - \langle{}^{0}\Psi^{\alpha,0}_{[n]}|\widehat{A}|{}^{0}\Psi^{\alpha,0}_{[n]}\rangle, \tag{B5}$$

as a direct consequence of Eq. (B4), by utilization of the fact that ${}^{\gamma}\Psi^{\alpha,\beta}_{[n]}$ is defined via the minimization of $\langle\Psi|\alpha\widehat{T}+\beta\widehat{V}_{ee}+\gamma\widehat{A}|\Psi\rangle$. Equation (B5) reduces to the Bauer relation for α=β=1. Using Eq. (B5) with $\widehat{A}=\widehat{T}$, they obtained for $T_{\rm xc}[n]$,

$$T_{\rm xc}[n]=\frac{\partial}{\partial\gamma}{}^{\gamma}E^{1,1}_{\rm xc}[n]\bigg|_{\gamma=0}=\frac{\partial}{\partial\gamma}{}^{\gamma}E^{1,1}_{c}[n]\bigg|_{\gamma=0}, \tag{B6}$$

where $T_{\rm xc}[n]$ is defined by

$$T_{\rm xc}[n]\equiv\langle{}^{0}\Psi^{1,1}_{[n]}|\widehat{T}|{}^{0}\Psi^{1,1}_{[n]}\rangle-\langle{}^{0}\Psi^{1,0}_{[n]}|\widehat{T}|{}^{0}\Psi^{1,0}_{[n]}\rangle, \tag{B7}$$

and the second equality in Eq. (B6) comes from the fact that the exchange part ${}^{\gamma}E^{1,1}_{x}[n]$ is independent of γ at zero temperature. The above relation (B7) is equivalent to the Bass equation,[35]

$$T_{\rm xc}[n]=a_B\frac{\partial^0E^{1,1}_{\rm xc}[n]}{\partial a_B}=a_B\frac{\partial^0E^{1,1}_{c}[n]}{\partial a_B}, \tag{B8}$$

which is the same as Eq. (97).

It is straightforward to generalize the above formalism to finite temperatures. Since we must average over all possible configurations of the system at nonzero temperatures, the expectation values in Eqs. (B1) and (B2) are changed

$$\langle{}^{\gamma}\Psi^{\alpha,0}_{[n]}|\cdots|{}^{\gamma}\Psi^{\alpha,0}_{[n]}\rangle\longrightarrow{\rm Tr}\,[e^{-\beta(\widehat{H}_0-\mu\widehat{N}-\Omega_0)}\cdots], \tag{B9}$$

$$\langle{}^{\gamma}\Psi^{\alpha,\beta}_{[n]}|\cdots|{}^{\gamma}\Psi^{\alpha,\beta}_{[n]}\rangle\longrightarrow{\rm Tr}\,[e^{-\beta(\widehat{H}-\mu\widehat{N}-\Omega)}\cdots], \tag{B10}$$

with

$$e^{-\beta\Omega_0}={\rm Tr}\,[e^{-\beta(\widehat{H}_0-\mu\widehat{N})}], \tag{B11}$$

$$e^{-\beta\Omega}={\rm Tr}\,[e^{-\beta(\widehat{H}-\mu\widehat{N})}], \tag{B12}$$

where $\widehat{H}_0=\alpha\widehat{T}+\gamma\widehat{A}$ and $\widehat{H}=\alpha\widehat{T}+\beta\widehat{V}_{ee}+\gamma\widehat{A}$. As in the zero-temperature case, the trace in Eq. (B9) depends on α, γ, and that in Eq. (B10) depends on α, β, and γ. Following the above argument for zero temperature, we obtain the exactly same relations (B5), (B6), and (B8) even at nonzero temperatures, with the corresponding replacements of (B9) and (B10).

However, we should have in mind that our definition of the exchange energy is different from that of many authors,[33–36] i.e., Eq. (B1) with α=β=1. Nevertheless, the combined definition (B4) is still correct with corresponding changes (B9) and (B10). Thus only the second equalities in Eqs. (B6) and (B8) become incorrect, so we obtain only the first equalities,

$$T_{\rm xc}[n]=\frac{\partial}{\partial\gamma}{}^{\gamma}E^{1,1}_{\rm xc}[n]\bigg|_{\gamma=0}=a_B\frac{\partial^0E^{1,1}_{\rm xc}[n]}{\partial a_B}. \tag{B13}$$

Furthermore, we obtain for our exchange-only scheme

$$T_{x}[n]=\frac{\partial}{\partial\gamma}{}^{\gamma}\mathcal{E}^{1,1}_{x}[n]\bigg|_{\gamma=0}=a_B\frac{\partial^0\mathcal{E}^{1,1}_{x}[n]}{\partial a_B}, \tag{B14}$$

where we used ${}^{\gamma}\mathcal{E}^{1,1}_{x}[n]$ to distinguish our definition of the exchange energy from others. Note that ${}^{0}E^{1,1}_{\rm xc}[n]$ is, in our notation, $\Omega_{\rm xc}$, and ${}^{0}\mathcal{E}^{1,1}_{x}[n]=\Omega_x(n,T)$.

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