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Free energy of the interacting electron gas including higher-order exchange effects

D. J. Kim

Department of Physics, Aoyama Gakuin University, Chitosedai, Setagaya, Tokyo, Japan*

Francis Bitter National Magnet Laboratory,† Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

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We discuss the free energy of an electron gas with the long-range Coulomb interaction by using the dielectric-response function which includes the higher-order exchange processes. Our result reproduces earlier results of Gell-Mann and Brueckner; Nozières and Pines; Hubbard; Englert and Brout; and others as special cases. The longitudinal spin-fluctuation effect is included in the present result, but its role seems to be significantly different from what is expected in the Hubbard-type model due to the large cross effect of the spin fluctuation and charge fluctuation even in the paramagnetic state.

I. INTRODUCTION

It is well known that the ground-state energy ($T=0$) or the free energy ($T>0$) of an electron gas can be related to the dielectric constant of the electron gas.[1,2] Recently we studied the dielectric response of an electron gas including the higher-order exchange processes.[3] In this paper we discuss the free energy of an electron gas by using the dielectric-response function that includes the effect of the higher-order exchange processes. One of the principal purposes of this paper is to expose the nature of the approximation included in our dielectric-response functions by comparing the free energy we derive with that of others. We find that in the zero-temperature limit our result reduces to the result of Hubbard[4] if a correspondence between his screened Coulomb interaction and our effective exchange interaction is assumed. Note that if the effect of the higher-order exchange processes is neglected the result of Hubbard reduces to that of Gell-Mann and Brueckner[5] and others. The above relation between our result and that of Hubbard and others seems to clarify the nature of the approximations contained in our dielectric response function. Since our discussion of the dielectric response can be naturally extended to the ferromagnetic state of the electron gas, we will be able to calculate the free energy of the electron gas in the ferromagnetic state in the same approximation as in the paramagnetic state.[6]

Thus the result in the present paper constitutes an extension of Hubbard's result to the finite temperature. There is, however, one important point we would like to emphasize in comparing our result with that of Hubbard. In our discussion we point out that the effective exchange interaction $\tilde{V}(q)$ appearing in our dielectric response function and accordingly in the free energy or ground-state energy is the same as that which produces the exchange enhancement of the paramagnetic susceptibility. This point about $\tilde{V}(q)$ leads us to a very interesting finding. The effect of the spin fluctuation in the strongly exchange-enhanced paramagnetic metals has been studied for the Hubbard-type short-range-interaction model and the spin-fluctuation effect was found to enhance the low-temperature electronic specific heat proportionally to the logarithm of the exchange enhancement factor.[7] In this paper we ask, what is the nature of the spin-fluctuation effect in the long-range Coulomb-interaction model? There is spin fluctuation in the long-range Coulomb model as well as in the Hubbard model. This can be seen from the fact that the paramagnetic susceptibilities of both models are essentially the same. But in the long-range Coulomb interaction model the contribution of the spin-fluctuation effect to the free energy seems to be significantly modified due to the interference of the spin fluctuation and charge fluctuation.

In Sec. II we review the dielectric-formulation method of calculating the free energy of the interacting electron gas. The charge (electron density) susceptibility including the higher-order exchange processes required in the calculation of the free energy is obtained in Sec. III. In Sec. IV the free energy is explicitly obtained using the result of Sec. III. Discussions of our results are given in Sec. V.

II. CALCULATION OF THE FREE ENERGY BY THE DIELECTRIC FORMULATION

The Hamiltonian of electrons including the long-range Coulomb interaction, imbedded in the uniform positive-charge background, is

$$\mathcal{H}=\sum_{l,\sigma}\epsilon_l c_{l\sigma}^\dagger c_{l\sigma}+\frac{1}{2}\sum_{\substack{l,l',\kappa;\\ \sigma,\sigma'}}{}' V(\kappa)c_{l\sigma}^\dagger c_{l'\sigma'}^\dagger c_{l'-\kappa,\sigma'}c_{l+\kappa,\sigma}, \tag{2.1}$$

where $c_{l\sigma}^\dagger$ is the creation operator of an electron at the state with energy ϵ_l and spin $\sigma(=+\text{or}-)$, $V(\kappa)$ is the Fourier transform of the Coulomb interaction

$$V(\kappa) = 4\pi e^2/\Omega\kappa^2, \tag{2.2}$$

where Ω is the volume of the system, and the prime on the summation indicates to exclude $\kappa = 0$ from the sum. It is well known that Eq. (2.1) can be rewritten as[8]

$$\mathcal{H} = \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} - \frac{1}{2}\frac{n}{\Omega}\sum_q V(q) + \frac{1}{2}\sum_q V(q)\rho(q)\rho(-q), \tag{2.3}$$

where n is the total number of electrons in the system and $\rho(q)$ is the Fourier transform of the electron density operator,

$$\rho(q) = \sum_k (c^\dagger_{k+} c_{k+q,+} + c^\dagger_{k-} c_{k+q,-}). \tag{2.4}$$

The second term in Eq. (2.3) is a constant and the essential part of the electron interaction is represented by the last term, which is of the form of density-density interaction.

Generally if we write the total Hamiltonian, which is the sum of the one-particle part $\mathcal{H}_0$ and the interaction $\mathcal{H}_{\text{int}}$, as a function of the coupling strength ξ,

$$\mathcal{H}(\xi) = \mathcal{H}_0 + \xi\mathcal{H}_{\text{int}} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}(\xi) \tag{2.5}$$

the free energy with the full interaction ($\xi = 1$), $F(1)$, is[2]

$$F(1) = F(0) + \int_0^1 \frac{1}{\xi}\langle\mathcal{H}_{\text{int}}(\xi)\rangle_\xi d\xi. \tag{2.6}$$

In Eq. (2.6), $F(0)$ is the free energy of the system without any interaction and $\langle A\rangle_\xi$ is the thermal average with the Hamiltonian $\mathcal{H}(\xi)$:

$$\langle A\rangle_\xi = \mathrm{Tr}(e^{-\beta\mathcal{H}(\xi)}A)/\mathrm{Tr}e^{-\beta\mathcal{H}(\xi)} \quad . \tag{2.7}$$

By applying Eq. (2.6) to the Hamiltonian Eq. (2.3) we obtain the expression for the free energy of the interacting electron gas,

$$F(1) = F(0) - \frac{1}{2}\frac{n}{\Omega}\sum_q V(q) + \frac{1}{2}\sum_q V(q)\int_0^1 d\xi\langle\rho(q)\rho(-q)\rangle_\xi \equiv F(0) - \frac{1}{2}\frac{n}{\Omega}\sum_q V(q) + \Delta F. \tag{2.8}$$

The contribution of the electron interaction to the free energy ΔF is given in terms of the electron-density fluctuation. By the general fluctuation-dissipation theorem[9] the electron-density fluctuation is related to the imaginary part of the electron-density response function. Using this fluctuation-dissipation theorem we rewrite ΔF, Eq. (2.8), in terms of electron-density response function.

First, we define the linear response of the electron density to a wave-number- and frequency-dependent external potential $\varphi(q, \omega)$ as

$$\chi_{ee}(q, \omega) = e\bar{\rho}(q, \omega)/\varphi(q, \omega), \tag{2.9}$$

where $\bar{\rho}(q, \omega)$ is the expectation of the electron density linear to the external potential. Thus defined, the charge susceptibility is given by the Kubo formula[9] as

$$\chi_{ee}(q, \omega) = e^2\frac{i}{\hbar}\int_0^\infty dt\, e^{i\omega t}\langle[\rho(q, t), \rho(-q)]\rangle \equiv e^2\chi'_{ee}(q, \omega), \tag{2.10}$$

where $[\ ,\ ]$ is the commutator, $\langle\cdots\rangle$ is the thermal expectation without the external potential, and $\rho(q, t)$ is given in the Heisenberg representation with the Hamiltonian which includes the electron interaction but not the external potential. Note that we can define $\chi_{ee}(q, \omega)_\xi$ simply by replacing $\langle\cdots\rangle_\xi$ in Eq. (2.10). Then by the fluctuation-dissipation theorem, the correlation of the electron density is given in terms of the imaginary part of the dynamical charge susceptibility:

$$\langle\rho(q)\rho(-q)\rangle_\xi = \frac{\hbar}{2\pi}\int_{-\infty}^\infty \coth\frac{\beta\hbar\omega}{2} \times \mathrm{Im}\,\chi'_{ee}(q, \omega + i0^+)_\xi\, d\omega. \tag{2.11}$$

Finally the free energy is obtained from Eqs. (2.8) and (2.11) as

$$\Delta F = \frac{\hbar}{4\pi}\sum_q V(q)\int_{-\infty}^\infty d\omega \coth\frac{\beta\hbar\omega}{2} \times \int_0^1 d\xi\, \mathrm{Im}\chi'_{ee}(q, \omega + i0^+)_\xi. \tag{2.12}$$

Note that Eq. (2.12) is an exact expression. Approximations are introduced only through the approximate calculation of the linear electron-density susceptibility $\chi_{ee}(q, \omega)_\xi$. Most of the previous calculation of the ground-state energy or free energy of the Coulomb electron gas used the ordinary random-phase approximation (RPA), which amounts to neglecting the higher-order exchange processes in calculating $\chi_{ee}(q, \omega)_\xi$. In Sec. III we calculate $\chi_{ee}(q, \omega)$ including the higher-order exchange processes.

III. DYNAMICAL CHARGE SUSCEPTIBILITY INCLUDING EXCHANGE EFFECTS

In calculating the charge susceptibility defined by Eq. (2.10) for the Hamiltonian Eq. (2.1) we note that $\chi'_{ee}(q, \omega + i0^+)$ is the Fourier transform of the following retarded double-time Green's function[10]:

$$\langle\rho(q, t)|\rho(-q)\rangle \equiv (i/\hbar)\langle[\rho(q, t), \rho(-q)]\rangle\theta(t), \tag{3.1}$$

where $\theta(t)$ is the step function

$$\theta(t) = \begin{cases} 1, & t > 0 \\ 0, & t < 0. \end{cases} \tag{3.2}$$

A standard way of obtaining the Green's function is to solve its equation of motion,

$$i\hbar\frac{\partial}{\partial t}\langle\rho(q,t)|\rho(-q)\rangle=-\delta(t)\langle[\rho(q),\rho(-q)]\rangle+\langle[\rho(q,t),\mathcal{H}]|\rho(-q)\rangle. \quad (3.3)$$

If we define the Fourier transform of the Green's function as

$$\langle\rho(q)|\rho(-q)\rangle_\omega=\int_{-\infty}^{\infty}\langle\rho(q,t)|\rho(-q)\rangle e^{i\omega t}\,dt, \quad (3.4)$$

the equation of motion can be rewritten as

$$\hbar\omega\langle\rho(q)|\rho(-q)\rangle_\omega=-\langle[\rho(q),\rho(-q)]\rangle+\langle[\rho(q),\mathcal{H}]|\rho(-q)\rangle_\omega. \quad (3.5)$$

Hereafter we investigate on the Fourier-transformed equation of motion, Eq. (3.5).

Corresponding to the following decomposition of the density operator,

$$\rho(q)=\rho^+(q)+\rho^-(q)=\sum_k[\rho_k^+(q)+\rho_k^-(q)], \quad (3.6)$$

where

$$\rho_k^\pm(q)=c_{k\pm}^\dagger c_{k+q,\pm}, \quad (3.7)$$

the Green's function can also be decomposed as

$$\langle\rho(q)|\rho(-q)\rangle_\omega=\sum_k[\langle\rho_k^+(q)|\rho(-q)\rangle_\omega+\langle\rho_k^-(q)|\rho(-q)\rangle_\omega]. \quad (3.8)$$

Corresponding to Eq. (3.5) we obtain the following form for the equation of motion:

$$\hbar\omega\langle\rho_k^+(q)|\rho(-q)\rangle_\omega=\langle[\rho_k^+(q),\ \rho(-q)]\rangle+\langle[\rho_k^+(q),\mathcal{H}_0+\mathcal{H}_c]|\rho(q)\rangle_\omega, \quad (3.9)$$

where we put $\mathcal{H}=\mathcal{H}_0+\mathcal{H}_c$, $\mathcal{H}_0$ and $\mathcal{H}_c$ being, respectively, the kinetic energy and the Coulomb interaction in Eq. (2.1). A similar equation can be obtained for $\langle\rho_k^-(q)|\rho(-q)\rangle_\omega$.

The commutators appearing in Eq. (3.9) are easily calculated:

$$[\rho_k^+(q),\ \rho(-q)]=c_{k+}^\dagger c_{k+}-c_{k+q,+}^\dagger c_{k+q,+}, \quad (3.10)$$

$$[\rho_k^+(q),\ \mathcal{H}_0]=(\epsilon_{k+q}-\epsilon_k)\,c_{k+}^\dagger c_{k+q,+}, \quad (3.11)$$

$$[\rho_k^+(q),\ \mathcal{H}_c]=\sum_{l,\kappa,\sigma}{}' V(\kappa)c_{k+}^\dagger c_{l\sigma}^\dagger c_{l-\kappa,\sigma}c_{k+q+\kappa,+}+\sum_{l,\kappa,\sigma}{}' V(\kappa)c_{l\sigma}^\dagger c_{k+\kappa,+}^\dagger c_{l+\kappa,\sigma}c_{k+q,+}. \quad (3.12)$$

By inserting Eqs. (3.10)–(3.12) into Eq. (3.9) we obtain

$$\hbar\omega\langle\rho_k^+(q)|\rho(-q)\rangle_\omega=(n_{k+q,+}-n_{k,+})+(\epsilon_{k+q}-\epsilon_k)\langle\rho_k^+(q)|\rho(-q)\rangle_\omega+\sum_{l,\kappa,\sigma}{}' V(\kappa)\langle c_{k+}^\dagger c_{l\sigma}^\dagger c_{l-\kappa,\sigma}c_{k+q+\kappa,+}|\rho(-q)\rangle_\omega+\sum_{l,\kappa,\sigma}{}' V(\kappa)\langle c_{l\sigma}^\dagger c_{k+\kappa,+}^\dagger c_{l+\kappa,\sigma}c_{k+q,+}|\rho(-q)\rangle_\omega, \quad (3.13)$$

where we put

$$\langle c_{k\sigma}^\dagger c_{k\sigma}\rangle=n_{k\sigma}. \quad (3.14)$$

The last two terms on the right-hand side of Eq. (3.13) are new Green's functions of more complicated structure than the original one. In order to reduce these higher-order Green's function to lower-order ones, we introduce the following approximations to the first term on the right-hand side of the commutator, Eq. (3.12):

$$\sum_{\kappa,l,\sigma}{}' V(\kappa)c_{k+}^\dagger c_{l\sigma}^\dagger c_{l-\kappa,\sigma}c_{k+q+\kappa,+}\cong\sum_{l,\sigma}V(-q)n_{k+}\,c_{l\sigma}^\dagger c_{l+q,\sigma}-\sum_\kappa{}' V(\kappa)n_{k+}c_{k+\kappa,+}^\dagger c_{k+\kappa+q,+}-\sum_\kappa{}' V(\kappa)n_{k+q+\kappa,+}\,c_{k+}^\dagger c_{k+q,+}. \quad (3.15)$$

The principle of the approximation in Eq. (3.15) is to retain only those terms which contain the diagonal number operators, such as $c_{k\sigma}^\dagger c_{k\sigma}$, and replace the number operator by their thermal expectation $n_{k\sigma}$. As will be seen later, the three terms on the right-hand side of Eq. (3.15) correspond, respectively, to the usual RPA term, the exchange-scattering term (which gives rise to the exchange enhancement of the paramagnetic susceptibility), and the exchange self-energy (which is responsible for the spin splitting of the bands in the ferromagnetic state).

The second term on the right-hand side of Eq. (3.12) can be approximated similarly to Eq. (3.15) as

$$\sum_{l,\kappa,\sigma}{}' V(\kappa)\,c_{l\sigma}^\dagger c_{k+\kappa,+}^\dagger c_{l+\kappa,\sigma}c_{k+q,+}\cong-\sum_{l,\sigma}V(q)n_{k+q,+}c_{l\sigma}^\dagger c_{l+q,\sigma}+\sum_\kappa{}' V(\kappa)n_{k+q,+}c_{k+\kappa,+}^\dagger c_{k+q+\kappa,+}+\sum_\kappa{}' V(\kappa)n_{k+\kappa,+}c_{k+}^\dagger c_{k+q,+}. \quad (3.16)$$

Further, the second terms on the right-hand side of Eqs. (3.15) and (3.16) can be simplified by introducing the effective exchange interaction $\tilde{V}(q)$ as follows:

$$\sum_\kappa{}' V(\kappa)c_{k+\kappa,+}^\dagger c_{k+q+\kappa,+}=\tilde{V}(q)\sum_\kappa c_{k+\kappa,+}^\dagger c_{k+\kappa+q,+}. \quad (3.17)$$

$\tilde{V}(q)$ defined in Eq. (3.17) should depend on k, but we neglect that dependence in what follows.

Inserting Eqs. (3.15), (3.16), and (3.17) into Eqs. (3.13) we obtain

$$(\hbar\omega+\tilde{\epsilon}_{k+}-\tilde{\epsilon}_{k+q,+})\langle\rho_k^+(q)|\rho(-q)\rangle_\omega=(n_{k+q,+}-n_{k,+})+V(q)\,(n_{k+}-n_{k+q,+})$$

$$\times[\langle\rho^+(q)|\rho(-q)\rangle_\omega+\langle\rho^-(q)|\rho(-q)\rangle_\omega] - \tilde{V}(q)(n_{k,+}-n_{k+q,+})\langle\rho^+(q)|\rho(-q)\rangle_\omega], \quad (3.18)$$

where we introduced the one-particle energy including the exchange self-energy $\tilde{\epsilon}_{k\sigma}$

$$\tilde{\epsilon}_{k\sigma}=\epsilon_k-\sum_\kappa{}' V(\kappa)n_{k+\kappa,\sigma}. \quad (3.19)$$

If we divide both sides of Eq. (3.18) and similar equations for $\langle\rho_k^-(q)|\rho(-q)\rangle_\omega$ by $(\hbar\omega+\tilde{\epsilon}_{k\pm}-\tilde{\epsilon}_{k+q,\pm})$ and sum over k, we obtain

$$\langle\rho^\pm(q)|\rho(-q)\rangle_\omega=F_\pm(q,\omega)-V(q)F_\pm(q,\omega)\times[\langle\rho^+(q)|\rho(-q)\rangle_\omega+\langle\rho^-(q)|\rho(-q)\rangle_\omega] + \tilde{V}(q)F_\pm(q,\omega)\langle\rho^\pm(q)|(-q)\rangle_\omega, \quad (3.20)$$

where $F_\pm(q,\omega)$ are the Lindhard functions of ± spin electrons:

$$F_\pm(q,\omega)=\sum_k\frac{n_{k+q,\pm}-n_{k,\pm}}{\tilde{\epsilon}_{k,\pm}-\tilde{\epsilon}_{k+q,\pm}+\hbar\omega} \quad (3.21)$$

By solving the coupled equation (3.20) we obtain the charge susceptibility

$$\chi'_{ee}(q,\omega)=\frac{1}{e^2}\chi_{ee}(q,\omega)=\langle\rho(q)|\rho(-q)\rangle_\omega$$

as

$$\chi'_{ee}(q,\omega)=\frac{\tilde{F}_+(q,\omega)+\tilde{F}_-(q,\omega)}{1+V(q)[\tilde{F}_+(q,\omega)+\tilde{F}_-(q,\omega)]}, \quad (3.22)$$

where we introduced the exchange-enhanced Lindhard function $\tilde{F}_\pm(q,\omega)$,

$$\tilde{F}_\pm(q,\omega)=\frac{F_\pm(q,\omega)}{1-\tilde{V}(q)F_\pm(q,\omega)}. \quad (3.23)$$

Note that Eq. (3.22) is valid for the ferromagnetic state of the electron gas as well as for the paramagnetic state. If we put $\omega=0$ in Eq. (3.22) it reduces to our earlier calculation of static charge susceptibility.[3] Essentially the same result as Eq. (3.22) was also obtained by Rajagopal *et al.*[11]

For the paramagnetic state Eq. (3.22) is simplified to

$$\chi'_{ee}(q,\omega)=\frac{2F(q,\omega)}{1+[2V(q)-\tilde{V}(q)]F(q,\omega)} \quad (3.24)$$

where $F(q,\omega)$ is the Lindhard function in the paramagnetic state which is spin independent,

$$F_+(q,\omega)=F_-(q,\omega)\equiv F(q,\omega). \quad (3.25)$$

If we put $\tilde{V}(q)=0$ in Eq. (3.24), it reduces to the RPA result.[12]

In order to illustrate the physical nature of the effective exchange interaction $\tilde{V}(q)$ let us consider the longitudinal magnetic susceptibility $\chi_{zz}(q,\omega)$ in the present model. If we use the Kubo formula the calculation of the magnetic susceptibility is quite parallel to the above calculation of the charge susceptibility. We encounter exactly the same commutator as Eq. (3.12) and if we employ exactly the same approximation to the commutator as above, we obtain

$$\chi_{zz}(q,\omega)=\mu_B^2\frac{\tilde{F}_+(q,\omega)+\tilde{F}_-(q,\omega)+4V(q)\tilde{F}_+(q,\omega)\tilde{F}_-(q,\omega)}{1+V(q)[\tilde{F}_+(q,\omega)+\tilde{F}_-(q,\omega)]}, \quad (3.26)$$

which in the paramagnetic state reduces to the familiar form[13]

$$\chi_{zz}(q,\omega)=\mu_B^2\frac{2F(q,\omega)}{1-\tilde{V}(q)F(q,\omega)}; \quad (3.27)$$

that is, the effective exchange interaction $\tilde{V}(q)$ appearing in the charge susceptibility is the same as that which appears in the denominator of the paramagnetic susceptibility. This fact is very important in our later discussions.

IV. FREE ENERGY OF THE INTERACTING ELECTRON GAS

We calculate the free energy of the electron gas by inserting Eq. (3.22) into Eq. (2.12). Note that $\chi'_{ee}(q,\omega)_\xi$ is obtained by replacing $V(q)$ and $\tilde{V}(q)$, respectively, by $\xi V(q)$ and $\xi\tilde{V}(q)$ in $\chi'_{ee}(q,\omega)$. Since our charge susceptibility, Eq. (3.22), is equally valid for the ferromagnetic state of the electron gas as well as for the paramagnetic state, we can calculate the free energy for both states by the same approximation. In the present paper, however, we will discuss only the free energy of the paramagnetic state by using the much simpler form of the charge susceptibility of the paramagnetic state, Eq. (3.24).

In carrying out the calculation of the free energy, we introduce the following simplification similar to Eq. (3.17):

$$\tilde{\epsilon}_{k\pm}=\epsilon_k-\sum_\kappa{}'V(\kappa)n_{k+\kappa,\pm}\equiv\epsilon_k-\tilde{V}(0)\sum_\kappa n_{k+\kappa,\pm}. \quad (4.1)$$

The $\tilde{V}(0)$ defined in Eq. (4.1) should depend on k but we neglect that dependence. Note that the approximation in Eq. (4.1) is consistent with that in Eq. (3.17). If we use the approximation in Eq. (4.1), $\chi'_{ee}(q,\omega)_\xi$ of the paramagnetic state takes the following simple form:

$$\chi'_{ee}(q,\omega)_\xi=\frac{2F(q,\omega)}{1+\xi[2V(q)-\tilde{V}(q)]F(q,\omega)}. \quad (4.2)$$

By putting Eq. (4.2) into Eq. (2.12) and carrying out the integration over ξ, we obtain the contribution of the electron interaction to the free energy,

$$\Delta F=\frac{\hbar}{2\pi}\sum_q\frac{V(q)}{2V(q)-\tilde{V}(q)}\int_{-\infty}^{\infty}d\omega\coth\frac{\beta\hbar\omega}{2}\times\mathrm{Im}\ln\{1+[2V(q)-\tilde{V}(q)]F(q,\omega+i0^+)\}. \quad (4.3)$$

Let us discuss how our result compares with the earlier results. If we put $\tilde{V}(q)=0$ in Eq. (4.3) it coincides exactly with the result of Englert and Brout,[2] which is the finite-temperature extension of the result of Nozières and Pines.[1] If we let the temperature go to zero, besides $\tilde{V}(q)=0$, in Eq. (4.3), it reduces to the result of Nozières and Pines.[2] Note that the result of Nozières and Pines is exactly the same as that of Gell-Mann and Brueckner[5] and others.

The inclusion of the higher-order exchange processes in calculating the ground-state energy of the electron gas with Coulomb interaction was first carried out by Hubbard.[4] At zero temperature our result coincides with that of Hubbard only if we assume the following form for the effective exchange interaction $\tilde{V}(q)$:

$$\tilde{V}(q)=4\pi e^2/\Omega(q^2+k_F^2) . \tag{4.4}$$

Therefore, our result, Eq. (4.3), can be regarded as the finite-temperature extension of the result of Hubbard.

Finally, let us point out again that we can calculate the free energy of the electron gas in the ferromagnetic state in the same approximation as in the paramagnetic state by using the charge susceptibility of the ferromagnetic state.

V. DISCUSSION: SPIN FLUCTUATIONS AND CHARGE FLUCTUATIONS

The effect of the spin fluctuation on the electronic specific heat in strongly exchange-enhanced paramagnetic metals has been discussed by using the Hubbard model or similar models which do not include the long-range part of the electron interaction.[7] The spin-fluctuation effect contribution to the free energy is most simply reproduced if we treat the Hubbard model[14] using the dielectric formulation:

$$\begin{aligned} F_H &= F_H(0)+\tfrac{1}{2}nU-\frac{\hbar}{2\pi}\sum_q\int_{-\infty}^{\infty}d\omega\,\coth\frac{\beta\hbar\omega}{2} \\ &\quad\times\frac{U}{N}\int_0^1 d\xi\,\mathrm{Im}\chi'_{-+}(q,\omega+i0^+)_\xi \\ &\equiv F_H(0)+\tfrac{1}{2}nU+\Delta F_H , \end{aligned} \tag{5.1}$$

where in the paramagnetic state, the transversal magnetic susceptibility in the Hubbard model is obtained by exactly the same approximation we used in Sec. III, as

$$\begin{aligned} \chi'_{-+}(q,\omega) &= (1/2\mu_B^2)\,\chi_{zz}(q,\omega) \\ &= \frac{F(q,\omega)}{1-(U/N)F(q,\omega)} \end{aligned} \tag{5.2}$$

In the above U is the repulsion between the electrons of opposite spins at the same atomic site, n is the total number of electrons, N is the total number of atomic sites in the system, and the subscript H stands for the Hubbard model. By putting Eq. (5.2) into Eq. (5.1) the spin-fluctuation effect contribution to the free energy is obtained:

$$\begin{aligned} \Delta F_H &= \frac{\hbar}{2\pi}\sum_q\int_{-\infty}^{\infty}d\omega\,\coth\frac{\beta\hbar\omega}{2} \\ &\quad\times\mathrm{Im}\ln[1-(U/N)F(q,\omega+i0^+)] . \end{aligned} \tag{5.3}$$

It was shown that ΔF_H gives rise to an enhancement of the electronic specific heat at low temperatures of the form $\gamma' T$, γ' being proportional to the logarithm of the exchange enhancement factor.

We can ask, what would be the corresponding effect of the spin fluctuation in the long-range Coulomb model? ΔF from Eq. (4.3), and ΔF_H from Eq. (5.3), have quite different analytical structure, especially for small q. In the following we answer this question.

According to the general theory of linear response,[9] the magnetic susceptibility is determined from the spectrum of the spin fluctuation of the system. Note that the magnetic susceptibilities calculated in the long-range Coulomb model and the Hubbard model are exactly the same if we identify the relation

$$\tilde{V}(q)=U/N \tag{5.4}$$

in Eqs. (3.27) and (5.2). Therefore, there must be essentially the same spectrum of spin fluctuations in the long-range Coulomb model as in the Hubbard model. We will show that actually a spin-fluctuation-effect contribution of the form of ΔF_H is included in our ΔF.

The logarithm in the integrand of Eq. (4.3) can be expanded and resummed as follows:

$$\begin{aligned} \Delta F &= \frac{\hbar}{2\pi}\sum_q g(q)\int_{-\infty}^{\infty}d\omega\,\coth\frac{\beta\hbar\omega}{2}\mathrm{Im}\ln[1+2V(q)F(q,\omega+i0^+)] \\ &\quad+\frac{\hbar}{2\pi}\sum_q g(q)\int_{-\infty}^{\infty}d\omega\,\coth\frac{\beta\hbar\omega}{2}\,\mathrm{Im}\ln[1-\tilde{V}(q)F(q,\omega+i0^+)] \\ &\quad+\frac{\hbar}{2\pi}\sum_q g(q)\int_{-\infty}^{\infty}d\omega\,\coth\frac{\beta\hbar\omega}{2}\,\mathrm{Im}[\text{cross terms of } V(q)F(q,\omega+i0^+) \text{ and } \tilde{V}(q)\,F(q,\omega+i0^+)] , \end{aligned} \tag{5.6}$$

where we put

$$g(q)\equiv V(q)/[2V(q)-\tilde{V}(q)] . \tag{5.7}$$

Note that $q(0)=\frac{1}{2}$ and it changes in the range from $q=0$ to $q\to\infty$ between $\frac{1}{2}$ and ~1. Thus $g(q)$ is a simple numerical factor on the order of 1.

There are three terms on the right-hand side of Eq. (5.6). The first term reduces to the result of Englert and Brout[2] if we assume $g(q)=\frac{1}{2}$; that is, it is the contribution of the charge (electron-density) fluctuation effect. If we put $g(q)=1$ and remember the correspondence Eq. (5.4), the second term is exactly the same as ΔF_H, Eq. (5.3); that is, the second term on the right-hand side of Eq. (5.6) represents a contribution from the spin-fluctuation effects. The third term can be naturally identified as the cross effects of the charge and spin fluctuations. As can be seen by comparing Eqs. (5.3) with (4.3), in the long-range Coulomb-interaction model this interference effect of the spin fluctuation and charge fluctuation plays a very important role even in the paramagnetic state and seems to modify significantly the contribution of the spin-fluctuation effect to the free energy. We will study this problem further in a separate paper.

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*Permanent address.

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[1]P. Nozières and D. Pines, Nuovo Cimento 9, 470 (1958).

[2]F. Englert and R. Brout, Phys. Rev. 120, 1085 (1960).

[3]D. J. Kim, H. C. Praddaude, and B. B. Schwartz, Phys. Rev. Lett. 23, 419 (1969); D. J. Kim, B. B. Schwartz, and H. C. Praddaude, Phys. Rev. B 7, 205 (1973).

[4]J. Hubbard, Proc. Roy. Soc. A 243, 336 (1957). For a related discussion, see L. Hedin and S. Lundquist, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1969), Vol. 23, p. 1.

[5]M. Gell-Mann and K. Brueckner, Phys. Rev. 106, 364 (1957). See also Ref. 8.

[6]L. Hedin, Phys. Rev. 139, A796 (1965). See especially Table II.

[7]N. Berk and J. R. Schrieffer, Phys. Rev. Lett. 17, 433 (1966); S. Doniach and S. Engelsberg, Phys. Rev. Lett. 17, 750 (1966). For many other references see J. R. Schrieffer, J. Appl. Phys. 39, 642 (1968).

[8]D. Pines, *Elementary Excitations in Solids* (Benjamin, New York, 1964).

[9]R. Kubo, J. Phys. Soc. Jap. 12, 570 (1957).

[10]D. N. Zubarev, Usp. Fiz. Nauk. 71, 71 (1960) [Soviet Phys. - Usp. 3, 320 (1960).

[11]A. K. Rajagopal, H. Brooks, and N. R. Ranganathan, Nuovo Cimento, Suppl. 5, 807 (1967).

[12]D. Pines and P. Nozières, *Theory of Quantum Liquids* (Benjamin, New York, 1966).

[13]T. Izuyama, D. J. Kim, and R. Kubo, J. Phys. Soc. Jap. 18, 1025 (1963).

[14]J. Hubbard, Proc. Roy. Soc. A 276, 238 (1963).