Renormalization constant and effective mass for the two-dimensional electron gas

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The renormalization constant and the effective mass for the two-dimensional (2D) interacting electron-gas system are determined as a function of density by evaluating the electron self-energy within the *GW* approximation. In order to investigate the effect of exchange-correlation interaction systematically, we have employed three types of model local-field correction factors in the dielectric function. We compare our results with those for the 3D electron gas. It is found that the renormalization constant for the 2D electron gas is smaller than that for the 3D system and the effective mass is greater in the 2D system, implying that the Coulomb interaction effect is more pronounced in the 2D than in the 3D system.

I. INTRODUCTION

There has been a great deal of interest in the two-dimensional (2D) electron systems[1] occurring at surfaces or interfaces of semiconductor materials. Since the electron concentration can be varied continuously and in a controlled manner over a wide range, these systems provide a useful testing ground for applying approximate methods of calculating the many-body properties of the system. Much interest in the 2D system arises from more recent origins. The fractional quantum Hall effect and the high-T_c superconductivity are believed to be 2D phenomena, which occur in the strongly interacting electron systems.

Recent angle-resolved photoemission spectroscopy (ARPES) studies for the the high-T_c superconductor[2] indicate that the quasiparticle weight becomes much enhanced near the Fermi level E_F, accompanied by a broad background, reflecting the Landau Fermi-liquid behavior. The quasiparticle weight at E_F, which is also called the renormalization constant Z_F, is interpreted as the amount of single-particle behavior of the particlelike excitations in the system. Thus it is equal to one for the noninteracting electron gas. For the interacting system, the quasiparticle weight becomes smaller than one due to the weight transfer to other multiparticle or collective excitations existing in the system. On the other hand, the renormalization constant determines the magnitude of the discontinuity in the momentum distribution function $n(\mathbf{k})$ at the Fermi surface (see Fig. 1) and so a *nonzero* renormalization constant implies the existence of the Fermi surface. Note that the renormalization constant is reduced to be zero in the Luttinger liquid model[3] or the marginal Fermi-liquid model,[4] proposed as possible models for the high-T_c superconductors.

Motivated by the above observation, we have attempted to determine the quasiparticle weight of the 2D electron gas to simulate quasiparticle excitations in the 2D strongly correlated system. The 2D electron gas in the low-density limit is expected to be an excellent model system for the strongly correlated 2D phenomena. We have calculated the renormalization constant for the 2D electron gas as a function of electron density. Results for the renormalization constant for the three-dimensional (3D) electron gas have been reported by several groups, whereas for the 2D electron gas, recent results by Santoro and Giuliani[5] only are available for a specific high-density regime. They used the *GW* approximation[6] with an effective interaction of Kukkonen and Overhauser.[7]

As to the effective mass for the 2D systems, Janak,[8] and Suzuki and Kawamoto[9] have evaluated it in the Si inversion layer using a static approximation to the screening, which neglects the frequency dependence of the dielectric function. Ting, Lee, and Quinn[10] have calculated the effective mass based on the random-phase approximation (RPA) and the Hubbard approximation (HA) to the dielectric function. They obtained the effective masses which are slightly larger than experimental values. Vinter[11] has performed calculations on the effective mass employing the plasmon-pole approximation to the dielectric function as suggested by Lundqvist[12] and by Overhauser.[13] Vinter used an effective-mass formula which is different from that used by Ting, Lee, and Quinn.[10] Their values were rather smaller than the experimental values. Recently, Santoro and Giuliani[5,14] have

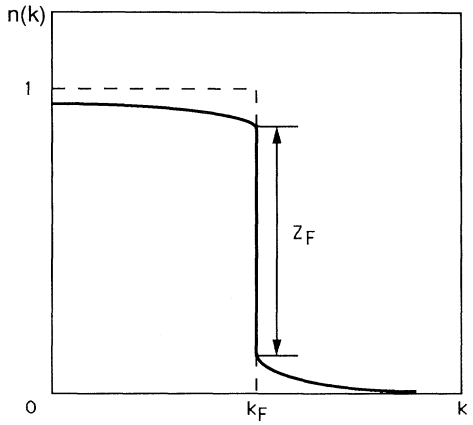

FIG. 1. Momentum distribution $n(k)$. The discontinuity at the Fermi surface corresponds to the renormalization constant.

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evaluated the effective mass, considering the frequency dependence of the electron self-energy including the vertex corrections induced by charge and spin fluctuation.

In this paper we have calculated the renormalization constant and the effective mass for an idealized 2D electron-gas system as a function of electron density, and compared them with existing results[15] for the 3D system. The electron self-energy is evaluated within the *GW* approximation. Correlation effects are systematically taken into account by employing three types of model local field correction factors in the dielectric function.

II. FORMALISM

We consider an idealized 2D electron-gas system, in which electrons are confined in a thin layer with a uniform positive neutralizing background charge and interact with each other through the Coulomb potential

$$v(\mathbf{q}) = \frac{2\pi e^2}{q}, \tag{1}$$

where $\mathbf{q}$ is a 2D wave vector. The dimensionless parameter characterizing such a 2D electron gas is the interelectron spacing r_s, which is defined by

$$\pi (r_s a_0)^2 = n^{-1}, \tag{2}$$

where a_0 is the Bohr radius and n is the surface electron density. The Fermi wave vector is expressed as

$$k_F = \sqrt{2\pi n} = (\alpha r_s a_0)^{-1}, \tag{3}$$

with $\alpha = 1/\sqrt{2}$. We take a special set of units in which $\hbar = m = 1$ and the momentum is measured in unit of the Fermi momentum ($k_F = 1$), and thus the Fermi energy $E_F = 1/2$. We measure the energy of the electron with respect to E_F, $\epsilon = E - E_F$.

The renormalization constant[16] is expressed as

$$Z_F = \left[1 - \frac{\partial}{\partial \epsilon} \mathrm{Re}\Sigma(\mathbf{k}, \epsilon)\right]^{-1}_{\mathrm{FS}}, \tag{4}$$

where $\Sigma(\mathbf{k}, \epsilon)$ is the *retarded* electron self-energy and FS represents that the calculation is done at the Fermi surface. As can be seen from the above equation, the renormalization constant is obtained from the energy dependence of the retarded electron self-energy.

In our system of units, the effective mass[17] can be expressed as

$$m^* = \left(1 - \frac{\partial \Sigma}{\partial \epsilon}\right)_{\mathrm{FS}} \left(1 + \frac{\partial \Sigma}{\partial k}\right)^{-1}_{\mathrm{FS}}. \tag{5}$$

The effective mass can be calculated from the energy and momentum dependence of the retarded electron self-energy.

In the *GW* approximation[6] the zero-temperature electron Matsubara self-energy is expressed as

$$\Sigma(\mathbf{k}, ik_n) = -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d^2q}{(2\pi)^2} \frac{v(\mathbf{q})}{\varepsilon(\mathbf{q}, i\omega)} \times g(\mathbf{k}+\mathbf{q}, ik_n + i\omega), \tag{6}$$

where $v(\mathbf{q})$ is the interaction potential, $\varepsilon(\mathbf{q}, i\omega)$ is the dielectric function, and $g(\mathbf{k}+\mathbf{q}, ik_n + i\omega)$ is the interacting Matsubara Green's function. In practical applications, one has often introduced a further approximation replacing g by a noninteracting Green's function g_0.

An approximate form of the dielectric function is commonly expressed as

$$\varepsilon(q, \omega) = 1 - \frac{v(q)\chi_0(q, \omega)}{1 + v(q) G(q, \omega) \chi_0(q, \omega)}, \tag{7}$$

where $\chi_0(q, \omega)$ is the noninteracting response function and $G(q, \omega)$ is the so-called local-field correction factor. For $\chi_0(q, \omega)$, we have used the form derived by Stern[18] for real values of ω and by Ting, Lee, and Quinn[10] for imaginary ω. The term $v(q)G(q, \omega)$ incorporates the effects of the exchange and correlation interaction in the dielectric function. In our study, we take a further approximation of using a static local-field correction factor; $G(q) = G(q, \omega = 0)$.

The simplest approximation to the local-field factor $G(q)$ is to take $G(q) = 0$, which corresponds to the random-phase approximation (RPA) where the short-range exchange-correlation interactions are neglected. The attempt to go beyond the RPA was made by Hubbard,[19] who obtained an explicit 3D expression of $G(q)$ using a diagrammatic approach. We take a 2D form of $G(q)$ which was derived by Jonson,[20]

$$G_{\mathrm{HA}}(q) = \frac{1}{2} \frac{q}{\sqrt{q^2 + k_F^2}}. \tag{8}$$

The Hubbard approximation (HA) takes into account the exchange interaction but neglects the correlation interaction.

As an attempt of including the correlation interaction, we also consider a modified Hubbard approximation (MHA), in which a model $G(q)$ of the 2D analog of the 3D form used by Rice[21] is adopted,

$$G_{\mathrm{MHA}}(q) = \frac{1}{2} \frac{q}{\sqrt{q^2 + k_F^2 + k_{\mathrm{TF}}^2}}, \tag{9}$$

where k_{TF} is the Thomas-Fermi wave vector. In the 2D electron gas, it is defined by

$$k_{\mathrm{TF}} = \frac{2\pi n e^2}{E_F} = \sqrt{2} r_s k_F. \tag{10}$$

In the MHA, the $G(q)$ has an explicit r_s dependence through k_{TF}. Furthermore, the compressibility sum rule is satisfied better in the MHA than in the HA. We expect that this r_s dependence embodies the correlation effects in some sense, so that the MHA gives better results for the physical properties than the HA.

The analytical continuation, $ik_n \rightarrow \epsilon + i\delta$, results in two terms for the *retarded* self-energy,[16]

$$\Sigma(\mathbf{k}, \epsilon) = \Sigma^{(\mathrm{line})}(\mathbf{k}, \epsilon) + \Sigma^{(\mathrm{res})}(\mathbf{k}, \epsilon), \tag{11}$$

with

$$\Sigma^{(\mathrm{line})}(\mathbf{k}, \epsilon) = -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d^2q}{(2\pi)^2} \frac{v(\mathbf{q})}{\varepsilon(\mathbf{q}, i\omega)} \times g_0(\mathbf{k}+\mathbf{q}, \epsilon + i\omega), \tag{12}$$

$$\Sigma^{(\mathrm{res})}(\mathbf{k},\epsilon) = \int \frac{d^2q}{(2\pi)^2} \frac{v(\mathbf{q})}{\varepsilon(\mathbf{q},\xi_{\mathbf{k}+\mathbf{q}}-\epsilon)} \times[\Theta(\epsilon-\xi_{\mathbf{k}+\mathbf{q}})-\Theta(-\xi_{\mathbf{k}+\mathbf{q}})], \quad (13)$$

where $\Theta(x)$ is the Heaviside step function, and $\Sigma^{(\mathrm{line})}(\mathbf{k},\epsilon)$ and $\Sigma^{(\mathrm{res})}(\mathbf{k},\epsilon)$ are called the line and residue part of the self-energy, respectively.

The derivatives of the self-energy with respect to momentum and energy are numerically obtained for given local-field correction factors.[22] Note that the derivative of the residue part of self-energy with respect to momentum vanishes at the Fermi surface.

III. RESULTS AND DISCUSSION

Results of numerical calculations for Z_F are given in Fig. 2 as a function of r_s. Results for the 3D system[15] are also provided for comparison. Three different types of local-field correction factors, RPA [$G(q) = 0$], HA [Eq. (8)], and MHA [Eq. (9)], are utilized in the calculations.

As shown in the figure, Z_F's for the 2D electron gas are substantially smaller than those for 3D system at the same value of r_s. This result can be understood from the fact that the interaction effect is stronger in 2D than in 3D so that electrons in the 2D system are more localized. Note, however, that the renormalization constants in the 2D system are *nonzero* even in the low-density region, which implies that, within our approximation scheme, the 2D electron-gas system is still the Fermi-liquid system as expected. As can be seen in the figure, the MHA result is smaller than the RPA one, but greater than the HA one. It seems that the exchange interaction, contained in the HA, makes the system more localized, but the correlation interaction, expected to be contained in the MHA, counteracts the role of the exchange interaction.

The density of high-T_c superconductors, if considered as a 2D homogeneous electron-gas system, corresponds to $r_s \sim 10$. The renormalization constant at this density turns out to be about 0.3. Thus, if high-T_c superconductors are described by 2D electron-gas systems, the quasiparticle spectral weight at E_F will become rather small, ~ 0.3, and a lot of weight will be transferred to the incoherent background.

In Fig. 3 effective masses m^* for the 2D electron gas are presented as a function of r_s, together with the corresponding 3D results[15] for comparison. Results by Rice[21] for the 3D system are also given. Rice also employed the MHA but used a different form of the dielectric function and a different formula for the effective mass from ours so that he obtained the effective masses which are a little bit smaller than ours of MHA.

As can be seen in the figure, m^*'s for the 2D electron gas are substantially larger than those for 3D at the same value of r_s. This result is again consistent with our results from the calculation of the renormalization constant that the interaction effect is stronger in 2D than in 3D so that electrons in the 2D system are more localized than in the 3D system. For both 2D and 3D systems, the effective masses are less than one at the very-high-density region (near $r_s = 0$) and monotonically increases as a function of r_s. This implies that the effect of $m_k[\equiv (1+\frac{\partial\Sigma}{\partial k})^{-1}_{\mathrm{FS}}]$, which gives rise to the mass reduction, is dominant near $r_s = 0$, but at the lower density region, the effect of $m_\epsilon[\equiv (1-\frac{\partial\Sigma}{\partial\epsilon})_{\mathrm{FS}}]$, which enhances the effective mass, dominates over the effect of m_k so that the product of the two becomes greater than one.[22] Thus at the densities of real metals ($r_s = 2 \sim 6$ for 3D), the effective mass m^* is greater than one. With increasing r_s, the potential energy becomes more sizable than the kinetic energy and so the electron system exhibits a more localized feature. The increase in m^* as a function of r_s is consistent with this trend.

One can see from Fig. 3 that results of the MHA and RPA are close to each other, whereas results of HA are the largest. As mentioned previously, the correlation interaction reduces the mass enhancement which is obtained with the exchange interaction only. Our results for the MHA are similar to recent results by Santoro and

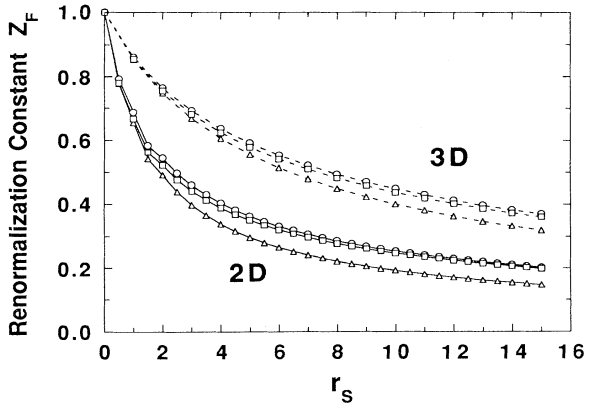

FIG. 2. The renormalization constant Z_F as a function of r_s. The solid lines denote results for the 2D electron gas and dotted lines for the 3D system. The open circles denote the RPA, the open triangles the HA, and the open squares the MHA.

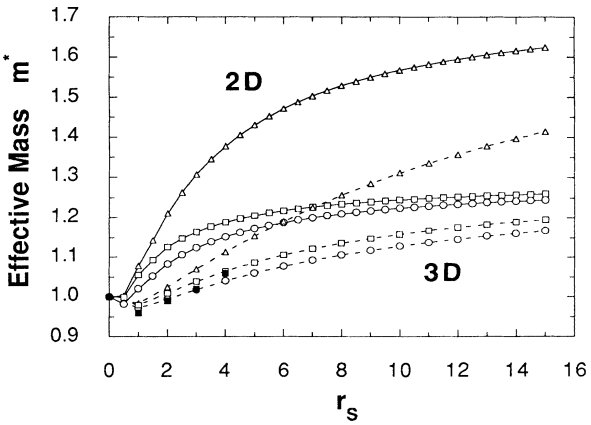

FIG. 3. The effective mass m^* as a function of r_s. The solid squares denote the results by Rice (Ref. 21) for the 3D system; other symbols are the same as those in Fig. 2.

Giuliani.[5,14] They calculated effective masses in the small r_s region, using much more complicated local-field correction factors associated with charge- and spin-fluctuations induced vertex corrections.

In summary, we have evaluated the renormalization constant and the effective masses in the 2D electron-gas system as a function of the electron density. The *GW* approximation for the electron self-energy is employed and the exchange-correlation interaction is considered via model local-field correction factors in the dielectric function. We have found that the renormalization constant is smaller in the 2D system than in the 3D system and the correlation effect reduces the effect of exchange interaction. We have found that the energy dependence of the self-energy plays a more important role in determining the effective masses than the momentum dependence of the self-energy does. We have also found that the effective mass is greater in the 2D system than in the 3D system, implying that the interaction effect is more prominent in the 2D than in the 3D system.

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