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Correlation in double-layer two-dimensional electron-gas systems: Singwi-Tosi-Land-Sjölander theory at $B = 0$

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We investigate the interaction effects for double-layer two-dimensional electron-gas systems in the absence of a magnetic field using both the random phase approximation (RPA) and Singwi-Tosi-Land-Sjölander (STLS) approximations. We show that the RPA overestimates correlation effects and that one needs, at a minimum, to include local-field corrections in order to get reliable estimates for the correlation energy and pair-distribution functions. The electron momentum distribution in double-layer systems is also studied by evaluating the electron self-energy from the screened exchange interaction. We find that RPA and STLS dielectric functions give quantitatively similar results for this quantity. The momentum distribution function depends very weakly on the layer separation of double-layer systems.

I. INTRODUCTION

Over the past three decades two-dimensional (2D) electron systems have been extensively studied both theoretically and experimentally.[1] Many properties of these systems are strongly influenced by the Coulombic electron-electron interactions.[2] Advances in the epitaxial growth of layered materials have recently made it possible to fabricate high-mobility double-layer 2D electron systems with electrons confined to nearby parallel planes separated by a distance comparable to the distance between electrons within a plane. These new systems exhibit a variety of qualitative effects due entirely to interlayer Coulomb interactions. In strong perpendicular magnetic fields where kinetic energies are quenched and interactions are most important new[3] fractional quantum Hall states appear because of interlayer correlations. Some of these states have a spontaneous broken symmetry associated with the layer degree of freedom which has recently attracted considerable attention.[4] Even in the absence of a magnetic field, however, new phenomena appear. Coulombic interlayer friction influences the transport properties[5] of double-layer systems. It has also been suggested that Wigner crystallization is favored for double-layer 2D electron systems[6] because of the interlayer electron interaction. In this article we present a study of the effect of interlayer correlations on some properties of double-layer electron-gas systems using approximations which are expected to be reliable at the densities of typical experimental systems.

Many-body effects for an interacting electron gas were first studied[7] using the random phase approximation (RPA). The RPA takes account of dynamic screening in the electron gas but does not include corrections due to exchange and correlation to the effective potentials associated with charge fluctuations in the system. The local-field theory[8,9] of Singwi, Tosi, Land, and Sjölander (STLS) includes these corrections in a simple physically motivated way and represents an important refinement of the RPA. As expected, corrections to the RPA are much more important in two dimensions than in three dimensions:[10] nevertheless comparisons of the STLS results with accurate Monte Carlo calculations[10,11] show that at least the ground state energy is given with remarkable accuracy by this simple approximation.

In this article we describe an application of the STLS approximation to double-layer 2D electron-electron and electron-hole systems. We calculate pair-correlation functions and ground state energies. We have also used the self-consistently determined dynamically screened interaction of the STLS approximation to evaluate the one-body Green's function from which we calculate the momentum distribution function. We have restricted ourselves to the case of zero magnetic field and to electron densities typical of experimental systems. In this regime the electrons form a weakly interacting system and the STLS approximation is believed to be reliable. (The STLS approximation has been applied to the strong magnetic field regime,[12] although its validity there is dubious.) We find that, as in the case of single-layer systems, the RPA gives a gross overestimate of correlation energies in double-layer systems. It is necessary to include local-field corrections to obtain reliable results for quantities like the electron pair distribution function and correlation energies, especially in the case of electron-hole double-layer systems. However, results for the electron momentum distribution do not depend strongly on whether the RPA or the STLS dielectric function is used. The dependence of the electron momentum distributions on interlayer interactions is surprisingly weak.

In the experimental systems which motivate these calculations electrons are confined to quantum wells and the layers have a finite width which is typically comparable to the electron-layer separation. If the subband separa-

tion in the quantum wells is large the finite width can be accounted for exactly by including appropriate form factors in the effective interlayer and intralayer Coulomb interactions. These finite width corrections for the electron layers are dependent on details of the geometry of a particular sample and for definiteness we restrict our attention in this article to the case of arbitrarily narrow electron layers. (For a single layer Jonson[10] found that corrections to the RPA were smaller in finite width systems.) The system is then completely specified by the layer separation and by the electron density in each layer. We employ effective atomic units so that the bulk dielectric constant and the effective mass of the semiconducting host appear only through their scaling of the effective Bohr radius: $a_B^* = \epsilon_B \hbar^2/m^* e^2$ and the Rydberg energy $\mathrm{Ry}^* = e^2/2a_B^*$. (For the conduction band of GaAs $a_B^* \sim 10$ nm.) The electron density in each layer will be expressed in terms of the customary dimensionless parameter r_s defined by $n^{-1} = \pi r_s^2 a_B^{*2}$. (For the conduction band of GaAs $n\,[10^{11}\ \mathrm{cm}^{-2}] \sim 3.2 r_s^{-2}$.)

The STLS approximation is based on a physically appealing picture, in which the static pair-distribution function is used to approximate short-range electronic correlations, rather than a systematic expansion in terms of a small parameter. Therefore there does not exist a simple parameter which can be used to quantify the accuracy of the STLS approximation. The validity of this approximation should ultimately be determined by comparing the calculated results to experimental data or to more sophisticated calculations, particularly Monte Carlo calculations. For single-layer two-dimensional systems this comparison indicates that the STLS approximation is remarkably accurate. In this paper we use the STLS approximation to estimate the importance of interlayer correlations for the experimentally relevent properties of a double-layer two-dimensional electron system within this approximation. The possibility that effects not accounted for by the STLS approximation may become noticeable under certain circumstance should be kept in mind.

In Sec. II we derive the self-consistent STLS equations for the correlation functions and density-density response functions appropriate for double-layer systems. Results for the pair-correlation functions and the correlation energies will be discussed in Sec. III and the calculations of the momentum distribution are described and the results presented in Sec. IV. Section V contains a summary of our results and a brief discussion of potential applications.

II. THE RPA AND STLS APPROXIMATIONS FOR DOUBLE LAYERS

The STLS theory is based on an approximation for the density-density response function χ, which is defined in the double-layer case by

$$\delta\rho_i(q,\omega) = \chi_{ij}(q,\omega) V_j^{\mathrm{ext}}(q,\omega), \tag{1}$$

where $i,j = L,R$ are layer indices and repeated indices are summed. In Eq. (1) $\delta\rho$ is the linear density response to the external perturbing field V^{ext}. $\chi(q,\omega)$ can be related formally to the dynamic density-density correlation function of the unperturbed system[13] but this cannot be evaluated exactly. The problem at hand is therefore to find a reliable approximation. In this section we briefly describe the application of the RPA and STLS approximations to double-layer systems.[14]

In both RPA and STLS approximations the system response to an external potential is equated with that of a noninteracting electron system responding to an external potential which includes an effective potential from the interaction with induced charges:

$$\delta\rho_i(q,\omega) = \chi_{ij}^0(q,\omega)[V_j^{\mathrm{ext}}(q,\omega) + V_j^{\mathrm{eff}}(q,\omega)]. \tag{2}$$

Here $\chi_{ij}^0 = \delta_{ij}\chi_i^0$ and χ_i^0 is the density-density response function of an isolated noninteracting 2D electron system with the density of layer i. χ_i^0 can can be evaluated analytically.[15] V^{eff} characterizes the effect of electron-electron interactions. The RPA and the STLS approximation differ in how V^{eff} is approximated. In the RPA, only the Hartree term of the electron-electron interaction is included so that $V_i^{\mathrm{eff}} = v_{ij}\delta\rho_j$, where the v_{ij} are the 2D electron-electron interaction potentials: $v_{LL}(q) = v_{RR}(q) = 2\pi e^2/q$ and $v_{LR}(q) = v_{RL}(q) = \exp(-qd)V_{LL}(q)$, where d is the separation between layers. The RPA does not account for correlations between the "responding electron" and the induced charge. To correct for this deficiency STLS (Ref. 8) introduced an exchange-correlation hole in the induced charge which was approximated using the *static, equilibrium* electron pair-distribution function.[16] For the two-layer case this ansatz leads to an effective interaction with the induced charge of the form

$$V_i^{\mathrm{eff}}(q,\omega) = v_{ij}(q)\delta\rho_j(q,\omega)[1 - G_{ij}(q)], \tag{3}$$

where the dependence of the local-field factors, $G_{ij}(q)$, on the pair-distribution functions $g_{ij}(\mathbf{r})$ is expressed through the static form factors (see below)

$$G_{ij}(q) = \frac{1}{n_j}\int \frac{d\mathbf{p}}{(2\pi)^2}\frac{\mathbf{q}\cdot\mathbf{p}}{qp}[\delta_{ij} - S_{ij}(\mathbf{p}-\mathbf{q})]e^{-|p-q|z_{ij}}, \tag{4}$$

where n_j is the average areal density of electrons in the jth layer, $z_{ij} = 0$ if $i = j$ and $z_{ij} = d$ if $i \neq j$. The derivation of Eq. (4) is straightforward following the spirit of the original STLS argument.[8]

Combining Eq. (2) and Eq. (3), we obtain the STLS expression for the density-density response function of a double-layer 2D electron gas system:

$$\chi^{-1}(q,\omega) = \begin{pmatrix} [\chi_L^0(q,\omega)]^{-1} - v_{LL}(q)[1 - G_{LL}(q)] & v_{LR}(q)[G_{LR}(q) - 1] \\ v_{RL}(q)[G_{RL}(q) - 1] & [\chi_R^0(q,\omega)]^{-1} - v_{RR}(q)[1 - G_{RR}(q)] \end{pmatrix}. \tag{5}$$

The RPA is recovered if the local-field factors are set to zero, i.e., $G_{ij}(q) \equiv 0$. The STLS approximation leads to a set of equations which need to be solved self-consistently. The static structure factors appearing in Eq. (4) which determine the local-field factors are related to equal time density-density correlations which in turn may be obtained by integrating the density-density response function over frequency using the zero-temperature fluctuation-dissipation theorem.[13] The integral over frequency must be done numerically and is most conveniently performed along the imaginary frequency axis where the response function is well behaved

$$S_{ij}(q) = -\frac{1}{n_i}\int_0^\infty \frac{d\omega}{\pi}\chi_{ij}(q,i\omega). \tag{6}$$

The great advantage of the analytical continuation of the response function to the complex frequency plane and the subsequent Wick rotation of the frequency integral is that it eliminates technical difficulties associated with the plasmon poles along the real frequency axis. Along the imaginary axis χ^0 is given by

$$\chi^0_{ii}(q,i\omega) = \frac{m^2}{\pi\hbar^2 q^2}\left\{\sqrt{2}\left[a+\sqrt{a^2+\left(\frac{q^2\omega}{m}\right)^2}\right]^{1/2} - \frac{q^2}{m}\right\} \tag{7}$$

with

$$a = \frac{q^4}{4m^2} - \frac{q^2 k_{Fi}^2}{m^2} - \omega^2. \tag{8}$$

Equations (4)–(6) comprise the STLS self-consistent equations for the double-layer system. Results obtained from the numerical solution of these equations are discussed in the next section.

Historically[17] the first attempt to go beyond the RPA in electron-gas calculations was the Hubbard approximation. This approximation may be obtained by using the Hartree-Fock approximation for the static structure factor in Eq. (4):

$$S^{\rm HF}_{ij}(q) = \delta_{ij}\begin{cases} \frac{2}{\pi}\sin^{-1}(q/2k_{Fi}) + q/(\pi k_{Fi})[1-(q/2k_{Fi})^2]^{1/2} & \text{if } q < 2k_{Fi} \\ 1 & \text{if } q > 2k_{Fi}. \end{cases} \tag{9}$$

The Hubbard approximation includes only exchange contributions to the local field and there is no local-field correction to the interlayer effective interaction. With the Hubbard approximation one is relieved from the task of solving the coupled STLS integral equations at the expense of neglecting the correlation contribution to the local field. In multilayer systems, the Pauli exclusion principle becomes less dominant, and we expect the Hubbard approximation to be less accurate than for a single-layer 2D electron system.

III. PAIR-DISTRIBUTION FUNCTIONS AND CORRELATION ENERGIES

Many properties of an electron-gas system are related to the frequency-dependent response function $\chi(\mathbf{q},\omega)$ obtained from self-consistently solving the coupled STLS equations. These properties can be separated into two categories. Quantities like the two-particle distribution function, the ground state energy, the collective excitation spectrum, etc., can be evaluated directly. Single-particle electron properties, like the quasiparticle lifetime, the quasiparticle effective mass, the momentum distribution function, etc., require the evaluation of the self-energy due to the Coulomb interaction between the particles. In this section we discuss only properties in the first category and delay to the next section a discussion of the evaluation of the self-energy and of interaction effects on single-particle electron properties. Although all the above-mentioned quantities can and have been calculated, we present results here only for the pair-distribution function and the ground state energy. These two quantities are chosen because they display correlation effects most clearly. The pair-distribution functions are calculated by performing a Fourier transform of the static structure factors which solve the STLS equations:

$$g_{ij}(\mathbf{r}) = n_j\int\frac{d^2q}{(2\pi)^2}[S_{ij}(\mathbf{q})-\delta_{ij}]\exp(i\mathbf{q}\cdot\mathbf{r}) . \tag{10}$$

The energy per particle of the electron-gas systems is conventionally separated into noninteracting, exchange, and correlation contributions. The electrostatic energy of the system is usually assumed to be zero because of the presence of a uniform neutralizing background and we follow that convention in this section. However, as we discuss briefly below, the electrostatic energy is important when considering response involving charge transfer between the layers. The exchange energy is the leading order term in the perturbative treatment of electron-electron interactions and may be determined by evaluating the expectation value of the interaction term in the Hamiltonian for the simple Fermi-sea Slater determinant. For the double-layer system both noninteracting and exchange energies are simply the sum of the corresponding energies for isolated 2D layers. The kinetic energy per particle is given by

$$t = \frac{1}{N_L+N_R}[N_L t^0(r_{sL}) + N_R t^0(r_{SR})], \tag{11}$$

where $t^0(r_s)$ is the kinetic energy per particle for an isolated layer:[2]

$$t^0(r_s) = 1/(n_\nu r_s^2). \tag{12}$$

In Eq. (12) n_ν is the valley degeneracy, i.e., the number of degenerate single-particle states per spin at each 2D wave vector. (For the conduction band of GaAs $n_\nu = 1$.) The exchange energy per electron is

$$\epsilon_x = \frac{1}{N_L + N_R}[N_L \epsilon_x^0(r_{sL}) + N_R \epsilon_x^0(r_{sR})], \tag{13}$$

where $\epsilon_x^0(r_s)$ is the exchange energy per electron for an isolated layer:[2]

$$\epsilon_x^0(r_s) = -\frac{8}{3\pi r_s}(2/n_\nu)^{1/2}. \tag{14}$$

The correlation energy is defined as the difference between the total ground state energy and the sum of the noninteracting and exchange contributions. We evaluate the ground state energy by using a coupling constant integration for the interaction term which requires that we be able to evaluate the expectation value of the interaction term in the Hamiltonian at any coupling strength. The necessary expectation values may be expressed in terms of the static structure factors and the correlation energy per particle is given by

$$\epsilon_c = \frac{1}{N_L + N_R}[N_L \epsilon_{cL} + N_R \epsilon_{cR} + N_L \epsilon_{cLR}]. \tag{15}$$

Here (in effective Rydberg energy units) the contributions to the correlation energy from the intra- and interlayer Coulomb interactions are, respectively,

$$\epsilon_{cL} = \left(\frac{2}{n_\nu}\right)^{1/2} \frac{1}{r_{sL} k_{FL}} \int_0^1 d\lambda \int_0^\infty dq\, [S_{LL}^{(\lambda)}(q) - S^{HF}(q)] \tag{16}$$

and

$$\epsilon_{cLR} = \left(\frac{2}{n_\nu}\right)^{1/2} \frac{1}{r_{sL} k_{FL}} \int_0^1 d\lambda \int_0^\infty dq\, e^{-qd}\, S_{LR}^{(\lambda)}(q). \tag{17}$$

$S^{(\lambda)}$ is the structure factor at a particular value of the coupling constant and the expression for ϵ_R is of the same form as that for ϵ_L. Equations (16) and (17) follow after noting that the exchange energy can be expressed in the form

$$\epsilon_x^0 = \left(\frac{2}{n_\nu}\right)^{1/2} \frac{1}{r_{sL} k_{FL}} \int_0^\infty dq\, [S^{HF}(q) - 1] \tag{18}$$

and that the Hartree-Fock static structure function is independent of coupling strength. Note that for large layer separations ϵ_{LR} goes to zero and the correlation energy is also the sum of contributions from the two independent layers. The correlation energy per particle goes to a constant at high densities ($r_s \ll 1$), while the kinetic energy and the exchange energy go like r_s^{-2} and r_s^{-1}, respectively, so the relative difference in total ground state energy between the RPA and the STLS approximations becomes insignificant at high densities. However, as we see below, quantitative corrections are important at densities for which high-mobility 2D systems can now be fabricated.

In Fig. 1 the correlation energy per particle is shown as a function of the particle density in each layer for both the RPA and the STLS approximation. The first thing to be noticed is that the magnitude of the correlation energy of the RPA is larger than the correlation energy of the STLS, roughly by a factor of 2. The overestimate of the correlation energy is a result of the fact that the RPA dielectric function does not incorporate effects of short-range correlations of the electrons. In the STLS approach, the local-field factors $G_{ij}(\mathbf{q})$ reduce the strength of the effective interaction potentials which enter the dielectric function. The overestimate of the correlation energy by the RPA is then essentially removed. As emphasized by Jonson,[10] the failure of the RPA is more dramatic in two dimensions than it is in three dimensions because of phase-space considerations which make short distances have a relatively larger importance. Figure 1 suggests that the basic conclusion of Jonson[10] that one has to go beyond the RPA in order to obtain a reasonably good description of correlation effects in 2D electron systems remains true for multilayer systems. In Fig. 2, the correlation energy per particle obtained from the STLS approximation is shown as a function of layer separations. At large layer separations the correlation energy equals that of two independent single layers. At zero layer separation, the double-layer system becomes equivalent to a single-layer system with a valley degeneracy $n_\nu = 2$. Our results in these two limiting cases agree with the results known from previous single-layer calculations.[10,11] As the layer separation increases, the correlation energy decreases smoothly, approaching the value that results for two independent layers when $d \geq K_F^{-1}$. This quantitative result suggests that interlayer correlations become important only at small layer separations.

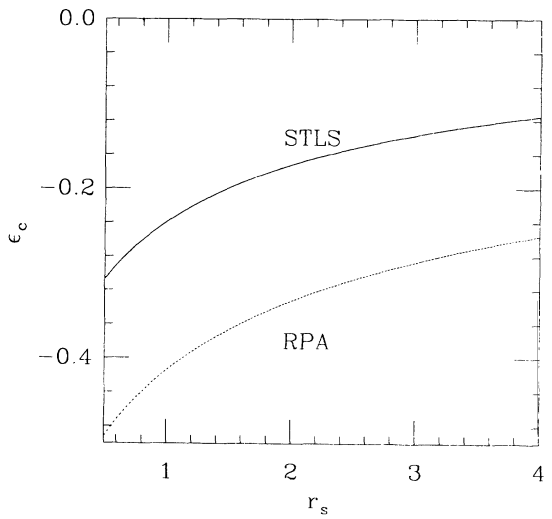

FIG. 1. Correlation energy per particle as a function of electron density in a double-layer system. The solid line is the STLS result and the dotted line is the RPA result. Results are shown for the case of equal layer densities and the layer separation at each density is $d = K_F^{-1}$.

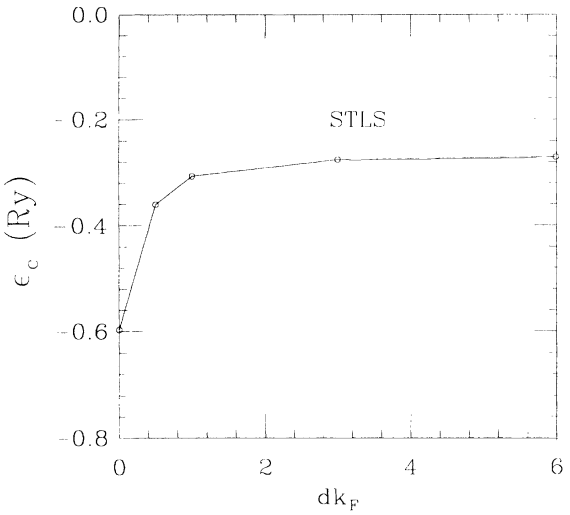

FIG. 2. Correlation energy per particle as a function of the layer separation in a double-layer system calculated from the STLS approximation. Two layers have equal density. Results are shown for $r_s = 0.5$. For GaAs this corresponds to $n \sim 1.3 \times 10^{12}$ cm^{-2} per layer. This density is higher than that of typical experimental samples.

In Fig. 3 the intra- and interlayer pair-distribution functions are shown for both the RPA and the STLS approximation. The difference between RPA and STLS approximation pair-distribution functions is consistent with the difference in their correlation energies. The correlation energy may be related to the interaction of an electron with its correlation hole which is described by the pair-distribution function. The failure of the RPA is most obviously manifested in Fig. 3 by the fact that the pair-distribution functions from the RPA fail to remain positive at small distances. This results in an overestimate of the exchange-correlation hole density at small distances and hence to an overestimate of the correlation energy. The STLS pair correlation has a very small violation of the positive requirement even for the fairly low density situation which is illustrated. Except in the case of very high electron densities, the STLS approximation is needed to obtain a reasonably accurate pair-distribution function. The interlayer correlation holes described by the interlayer pair-distribution function will diminish quickly at large layer separations ($d \geq K_F^{-1}$). As mentioned earlier, the Hubbard approximation cannot include the effect of interlayer correlation. It is therefore expected to be a poorer approximation in a multilayer system than for a single-layer 2D electron gas.

In electron-hole double-layer structures, where one layer contains a 2D electron gas and the other contains a 2D hole gas, the RPA results are even less reliable. This is no surprise since mean-field theories like the RPA are expected to be especially poor for attractive interactions. In Fig. 4 the pair distribution functions of an electron-hole double layer are shown for both the RPA and the STLS approximation. One can see clearly that the interlayer correlation from the STLS is much stronger than that from the RPA. To obtain reliable results for the electron-hole double-layer system, it is especially necessary to go beyond the RPA.

IV. SELF-ENERGY AND THE MOMENTUM DISTRIBUTION FUNCTION

Single-particle properties of the 2D electron layers are obtained from a calculation of the self-energy due to electron-electron interaction. In this section we describe a self-energy calculation based on the STLS approximation for the dynamically screened electron-electron interaction. This approximation we use does not predict

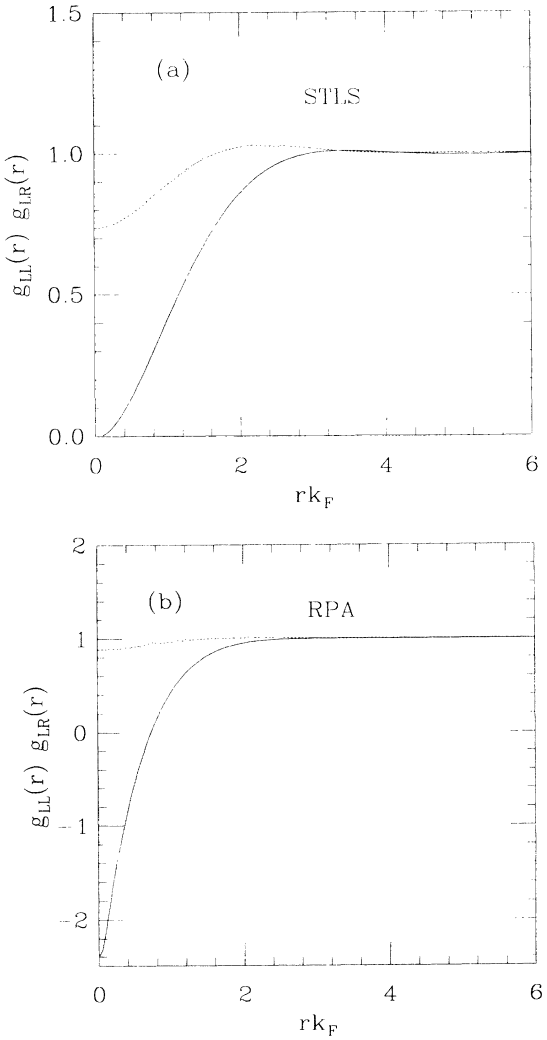

FIG. 3. The intralayer (solid line) and interlayer (dotted line) electron pair-distribution functions in a double-layer system calculated from the STLS (a) approximation and the RPA (b). The two layers have the same electron. Results are shown for $r_s = 4$. For GaAs this corresponds to $n \sim 2.0 \times 10^{10}$ cm^{-2} per layer. This density is close to the lowest at which high mobility samples can presently be fabricated. The layer separation is $d = K_F^{-1} \sim 28$ nm.

any violations of Fermi liquid theory; the possibility of such violations in 2D electron systems has recently been the subject of speculations motivated by the unusual electronic properties of the conducting planes of high-temperature superconductors.[18] The conditions (if any) under which violations of Fermi liquid occur in 2D systems are not known and we appeal to the absence of any experimental indication of violations in the 2D electron-gas case to justify our approach. The assumption of the Fermi liquid picture for the electron gases implies that interaction effects will not change the single-particle electron properties qualitatively, although important quantitative effects can occur.

We approximate the self-energy by a single term describing the dynamically screened interaction of an electron with its exchange hole. When the RPA is used to determine the screened interaction the result is the RPA approximation for the self-energy which, from a perturbation theory point of view, is a sum of ring diagrams.[13] The local-field factors $G(\mathbf{q})$ which appear in the STLS approximation for the dielectric function can be viewed as approximating vertex corrections to the polarization loops in the RPA ring diagrams. In this section, we first sketch the procedure for evaluating the self-energy, and then discuss the momentum distribution of the electrons which results. As in the preceding section, the results from the RPA and the STLS approximation will be compared and the dependence of the momentum distribution on electron densities and on layer separations will be illustrated. Although other single-particle electron properties can also be determined once the self-energy is evaluated, we concentrate here on the momentum distribution.

When there is no hopping of electrons between the two layers, the particle number in each layer is a constant of the motion and the electron Green's function must be diagonal with respect to the layer indices. We may split the self-energy into exchange and correlation parts: $\Sigma_{LL} = \Sigma^x_{LL} + \Sigma^c_{LL}$ where the exchange self-energy is obtained without including screening and the correlation self-energy is defined by this equation. The exchange self-energy for one layer is real, independent of frequency, independent of the presence of the other layer, and reducible to a simple integral.[19,20] In effective Rydberg units, it is given by

$$\Sigma^x_{ii}(k) = -\frac{2}{r_{si}}\left(\frac{2}{n_\nu}\right)^{1/2}\left[1 - \frac{1}{\pi}\int_{|k_{Fi}-k|}^{k+k_{Fi}} \sin^{-1}\left(\frac{k^2+q^2-k_{Fi}^2}{2kq}\right)\frac{dq}{k_{Fi}}\right]. \tag{19}$$

The correlation contribution to the self-energy has the usual branch cut along the real frequency axis.[13] We evaluate the retarded self-energy $\Sigma^c_{LL}(k, ip_n = \omega + i0^+)$. Since the real part and imaginary parts of Σ^c_{LL} satisfy Kronig-Kramers relations it is sufficient to evaluate the imaginary part of this quantity.

In the Matsubara formalism, the approximation we employ for the self-energy is given by

$$\Sigma_{LL}(k, ip_n) = -\frac{1}{\nu}\sum_{\mathbf{q}}\frac{1}{\beta}\sum_{i\omega_n} v^{\rm scr}_{LL}(q, i\omega_n) \times \mathcal{G}^0_{LL}(\mathbf{q}+\mathbf{k}, i\omega_n + ip_n), \tag{20}$$

where ν is the area of the 2D layers and $v^{\rm scr}_{LL}$ represents a screened intralayer interacting potential for which an explicit expression will be given in the following. To motivate our expression for $v^{\rm scr}_{LL}$, we rewrite Eq. (5) in the following form:

$$\chi = [1 - \chi^0 \Gamma V]^{-1}\chi^0\Gamma. \tag{21}$$

Here each variable is a 2×2 matrix with respect to the layer index. χ^0 is the diagonal 2×2 matrix specifying the independent response of two noninteracting two-dimensional layers. V has as its elements v_{ij}, the bare Coulomb potentials between two electrons in the ith and jth layers. The quantity Γ is defined by Eq. (21); it may be interpreted as approximating vertex corrections to the polarization loops of the RPA. Comparing Eq. (21) and Eq. (5) we see that Γ is related to the local-field factors $G(\mathbf{q})$ by

$$\Gamma^{-1}(\mathbf{q}) = 1 + U\chi^0 \tag{22}$$

with the elements of U defined by

$$u_{ij}(\mathbf{q}) = v_{ij}(q)G_{ij}(\mathbf{q}). \tag{23}$$

The approximation we use for the screened electron-electron interaction potential is

$$\begin{aligned} V^{\rm scr}(q,\omega) &= \Gamma(q)\epsilon(q,\omega)^{-1}V(q) \\ &= \Gamma(q)[1 + V(q)\chi(q,\omega)]V(q) \\ &= [1 - \chi^0(V-U)]^{-1}V. \end{aligned} \tag{24}$$

This particular form is motivated by identification of Γ as an approximate vertex correction and requires the insertion of the same approximate vertex correction in the self-energy diagram as in the polarization loops. (See, for example, the corresponding discussion for single component systems in Ref. 13.) The explicit form for the screened intralayer electron-electron interaction potential is obtained by inverting the necessary 2×2 matrices to obtain the diagonal elements of $V^{\rm scr}$:

$$v^{\rm scr}_{RR}(q,\omega) = \frac{[1 - v_{LL}(1-G_{LL})\chi^0_{LL}]v_{LL} + v^2_{LR}(1-G_{LR})\chi^0_{RR}}{[1-\chi^0_{LL}v_{LL}(1-G_{LL})][1 - v_{RR}\chi^0_{RR}(1-G_{RR})] - [v_{LR}(1-G_{LR})]^2\chi^0_{LL}\chi^0_{RR}}. \tag{25}$$

The RPA is recovered by setting all the local-field corrections to zero; $G_{ij}(q) = 0$. For the STLS approximation, the $G_{ij}(q)$ are obtained by solving the self-consistent STLS equations in the previous sections.

Performing the analytical continuation on Eq. (20), we get the imaginary part of the retarded self-energy as[13]

$$\mathrm{Im}\Sigma^{c}_{LL}(k,\omega) = \frac{1}{\nu}\sum_{\mathbf{q}} \mathrm{Im}[v^{\mathrm{scr}}_{LL}(q,\xi^{0}_{\mathbf{k}+\mathbf{q}}-\omega)] \times[\theta(\omega-\xi^{0}_{\mathbf{k}+\mathbf{q}})-\theta(-\xi^{0}_{\mathbf{k}+\mathbf{q}})], \quad (26)$$

where energies are measured from the Fermi energy. From the above expression we can see immediately that $\mathrm{Im}[\Sigma^{c}_{LL}(\omega=0)]=0$, so the electron lifetime at the Fermi surface is infinite. It is important in the above expression to include the contribution from the plasmon poles in the screened interaction which occur along the real frequency axis. (Both the real and imaginary parts of the denominator of Eq. (25) vanish at both in-phase and out-of-phase plasmon frequencies and $\mathrm{Im}[v^{\mathrm{scr}}_{LL}]$ has a δ-function contribution which must be included.) With Eqs. (25) and (26), the imaginary part of the retarded self-energy can be computed numerically. Employing the Kronig-Kramers relations, the real part of the correlation self-energy can then be evaluated.

Combining the above numerically obtained results with Eq. (19) gives a complete result for the one-body Green's function and we are then able to evaluate any single-electron property of the system. In particular, the momentum distribution for the electrons is[13] given by

$$n(k) = \int_{-\infty}^{0} \frac{d\omega}{2\pi} A(k,\omega), \quad (27)$$

where the spectral function is related to the self-energy by

$$A(k,\omega) = -2\mathrm{Im}\frac{1}{\omega+i0^{+}-\xi^{0}_{k}-\Sigma^{\mathrm{ret}}_{LL}(k,\omega)}. \quad (28)$$

The size of the discontinuity of the electron momentum distribution function at the Fermi surface, denoted by Z_F, provides a direct measure of the interaction effects. For a free electron gas, $Z_F = 1$, while for an interacting electron gas $0 \le Z_F \le 1$. This quantity, the quasiparticle renormalization constant, is related to the self-energy by[13]

$$Z_F = \frac{1}{\left[1-\partial\mathrm{Re}\Sigma^{\mathrm{ret}}_{LL}(k,\omega)/\partial\omega|_{k=k_F\ \omega=0}\right]}. \quad (29)$$

The momentum distribution function of the electrons calculated from the STLS dielectric function is shown in Fig. 5 for two different electron densities. Decreasing

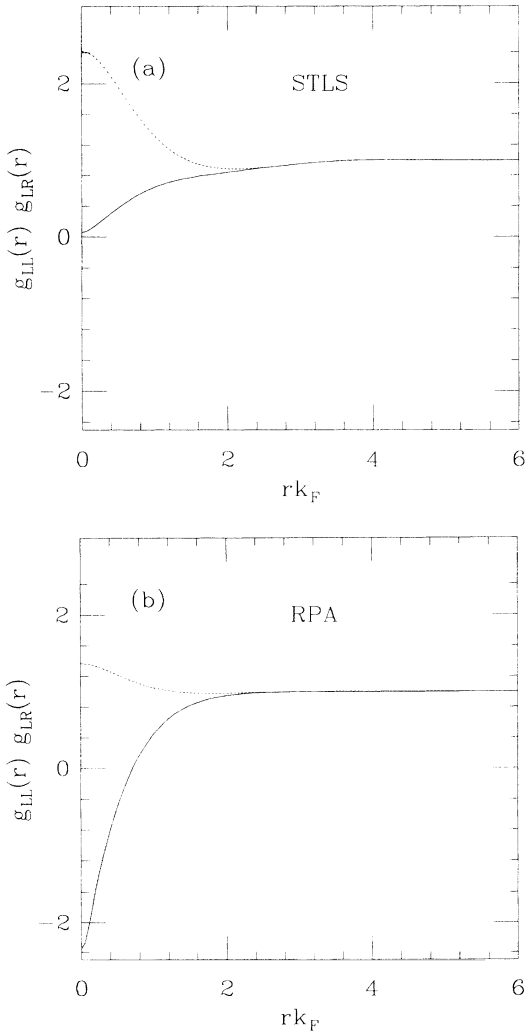

FIG. 4. The intralayer (solid line) and interlayer (dotted line) particle pair-distribution functions in an electron-hole double-layer system calculated from the STLS (a) and the RPA (b). The two layers have equal carrier densities with density parameter $r_s = 4$ and the electron and hole masses were taken to be equal. The layer separation is $d = 0.5\ K_F^{-1}$ as in Fig. 3.

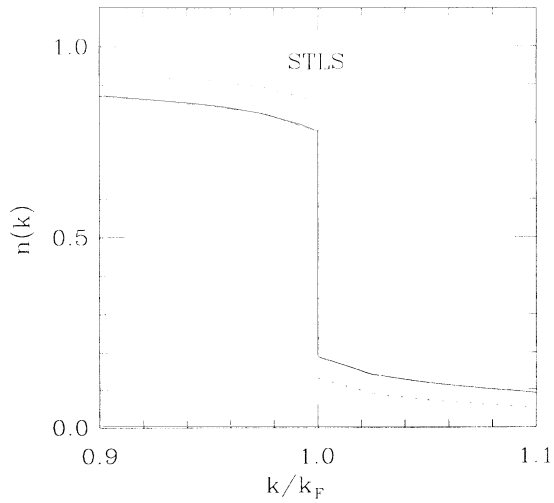

FIG. 5. Electron momentum distributions in a double-layer system calculated from the STLS approximation with $r_s = 1$ (dotted line) and $r_s = 2$ (solid line). ($n \sim 3.2 \times 10^{11}$ cm^{-2} and $n \sim 0.8 \times 10^{11}$ cm^{-2}.) The layer separation in each case is $d = K_F^{-1}$. ($d \sim 7$ nm and $d \sim 14$ nm.) The layers have equal electron density.

the density will increase the interaction effect and reduce the discontinuity at the Fermi surface Z_F. In Fig. 5, the values of Z_F are about 0.7 and 0.6 for the densities of $r_s = 1$ and $r_s = 2$, so the electron momentum distributions have not departed much from the case of free electrons. The difference in the electron momentum distribution between using the RPA and the STLS dielectric functions is also examined. The result is shown in Fig 6. Unlike the case of the correlation energy and pair-distribution function, where the RPA overestimates the correlation effects tremendously, the difference between using the RPA and the STLS dielectric functions in the momentum distribution is small. In the inset of Fig. 6, $\mathrm{Re}\Sigma^{\mathrm{ret}}_{LL}(\omega)$ is shown as a function of ω. We can see that the values of $\Sigma^{\mathrm{ret}}_{LL}$ at $\omega = 0$ for the RPA and the STLS approximation differ noticeably, the correlation energies per particle differ accordingly. However, the values of $\partial \mathrm{Re}\Sigma^{\mathrm{ret}}_{LL}(w)/\partial\omega$ at $\omega = 0$ from the RPA and the STLS are almost the same. Since Z_F depends only on the value of the derivative, the difference of the momentum distribution between the RPA and the STLS approximation is not noticeable. Earlier calculations for the single-layer 2D electron gas also show that the values of Z_F from the RPA and Hubbard approximations are almost the same.[21] In Fig. 7, the momentum distributions calculated from the STLS dielectric function for different layer separations are shown. The dependence of the electron momentum distribution on the layer separation is weak. When the layer separation is reduced, the Coulomb interaction potential increases, as does the typical screening strength. Therefore the overall influence of the layer separation on the electron momentum distribution, as shown in Fig. 7, is weak.

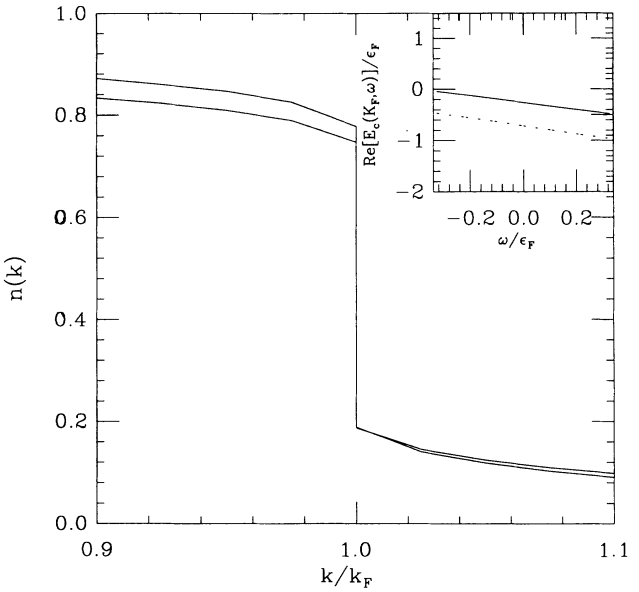

FIG. 6. Electron momentum distributions in a double-layer system calculated from the STLS approximation (dotted line) and the RPA (solid line). The layer separation is $d = K_F^{-1}$. The two layers have the same electron density with $r_s = 2$. The inset shows the real part of the self-energies, not including the exchange energy, as a function of the frequency ω for the STLS approximation (dotted line) and the RPA (solid line).

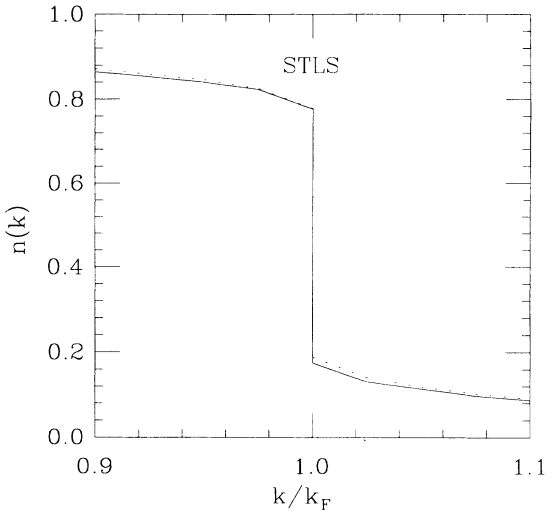

FIG. 7. Electron momentum distributions in a double-layer system calculated from the STLS approximation for layer separations of $d = K_F^{-1}$ (dotted line) and $d = 0.3\ K_F^{-1}$ (solid line). The two layers have the same electron density with $r_s = 2$.

V. SUMMARY

The STLS approximation provides a reasonably accurate quantitative description of interaction effects in double-layer 2D electron systems. Solving the self-consistent STLS equations for the dynamic screening function numerically leads directly to estimates of correlation effects on quantities such as the pair-correlation function and the ground state energy. Single-electron properties can be obtained by evaluating the self-energy using the STLS dielectric function. This enables one to calculate interaction effects on additional experimentally observable quantities. In this article, we have investigated interaction effects for the 2D electron systems in a double-layer structure in the absence of magnetic field. We have considered both the RPA and the self-consistent STLS approximation. Our calculations show that the RPA badly overestimates correlation effects for interacting double-layer 2D electron systems. Except at very high densities it is necessary to employ the STLS scheme in order to obtain reliable results for the correlation energy and pair-distribution function. These results have measurable consequences. For example, the density dependence of the correlation energies in the double-layer sytems can be measured by studying the capacitance of the double-layer structure[22] and the interlayer friction[5] is proportional to an average of the square of the screened interlayer interaction.

The electron momentum distribution in double-layer systems has also been studied by evaluating the electron self-energy from the screened exchange interaction. We find that the RPA and the STLS dielectric functions give quantitatively similar results for the electron momentum distributions. The results also show that the momentum

distributions depend very weakly on layer separations in double-layer systems, except possibly at very small layer separations.

In this article we have presented some numerical results for layer separations which cover the range of densities and layer separations of typical experimental systems. In order to compare with measurements on a particular system it is necessary to account in detail for the geometry of that system including the finite width of both quantum wells. The calculations described here[23] can then be carried out without any essential modification for any sample geometry.

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