Correlations in coupled electron and hole layers of finite thickness

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The variational multicomponent hypernetted-chain scheme for the double-layer electron-electron and electron-hole systems developed by us is generalized to the case where the layers have finite thickness. We have also studied the elementary collective excitations and the region of stability of these systems as the layer separation is varied. In a single electron layer our result for the bulk modulus is in good agreement with the available experimental results.

Double layers of two-dimensional (2D) electron and hole systems have recently been a subject of intense research, because of the novel physical phenomena detected in these systems. Most of these phenomena are related to the quantum Hall effect,[1] but the double electron layer system has also been used in the measurement of the compressibility of a single electron gas layer.[2] Since the advanced epitaxial growth techniques have made it possible to fabricate double-layer systems, where the interlayer separation is comparable to the distance between electrons within one plane, the understanding of interlayer interactions has become important. These interactions are responsible for the new fractional quantum Hall (FQH) states,[1,3] and also in the absence of magnetic field may cause phenomena like possible enhancement of the Wigner crystallization.[4]

In this paper, we report our studies of coupled electron-electron and electron-hole layer systems at zero magnetic field. We extend our earlier model, which has been shown[5] to be an efficient tool when studying the layered electron (or hole) systems, to the case of layers with finite thickness. As a starting point, we use the Jastrow variational wave function for the multicomponent system:

$$\Psi = \left\{ \prod_{\alpha=1}^{M} \Phi_\alpha \prod_{i<j\le N_\alpha} f_{\alpha\alpha}(r_i^\alpha - r_j^\alpha) \right\} \times \left\{ \prod_{\alpha<\beta\le M} \prod_{i=1}^{N_\alpha} \prod_{j=1}^{N_\beta} f_{\alpha\beta}(r_i^\alpha - r_j^\beta) \right\}, \tag{1}$$

where Φ_α is the wave function of N_α noninteracting particles of species α. All correlation effects are included in the functions $f_{\alpha\beta}$. Using this wave function and the hypernetted-chain (HNC) approximation, one can calculate the total energy of the system[5] and also derive the Euler-Lagrange equations for the pair-correlation functions $g_{\alpha\beta}(\mathbf{r})$,

$$\frac{-\hbar^2}{2m_{\alpha\beta}} \nabla^2 [g_{\alpha\beta}(\mathbf{r})^{1/2}] + [V_{\alpha\beta}(\mathbf{r}) + w_{\alpha\beta}(\mathbf{r})][g_{\alpha\beta}(\mathbf{r})]^{1/2} = 0, \tag{2}$$

where the functions $w_{\alpha\beta}(\mathbf{r})$ are the elements of the matrix whose Fourier transform is

$$w(\mathbf{q}) = \frac{-\hbar^2 q^2}{4} \{ [S(\mathbf{q}) M S(\mathbf{q})]^{-1} - [S_F(\mathbf{q}) M S_F(\mathbf{q})]^{-1} + M^{-1}[S(\mathbf{q}) - 1] + [S(\mathbf{q}) - 1] M^{-1} \}. \tag{3}$$

The structure functions $S_{\alpha\beta}(\mathbf{q})$ are obtained as Fourier transforms of $g_{\alpha\beta}(\mathbf{r})$. In practice, we cast the above equations into a k-space form, which is then solved iteratively, using the uncorrelated case as a starting point.[5]

So far, the layers have been assumed to be strictly two-dimensional and, therefore, the interparticle potential of the form

$$V_{\alpha\beta}(r) = \frac{e^2}{\sqrt{r^2 + |\alpha - \beta|^2 c^2}} \tag{4}$$

has been used. Here, α and β are layer indices and c is the separation between the layers. The finite thickness of the layers is modeled by using the Fang-Howard variational wave function,[6]

$$g(z) = \frac{1}{2} b^3 z^2 e^{-bz}, \tag{5}$$

where z is the coordinate axis perpendicular to the layers. The optimum value of the variational parameter b is given by

$$b = (33\pi m^* e^2 n / 2\epsilon\hbar^2)^{1/3}, \tag{6}$$

where $m^* = 0.067 m_e$ is the electron effective mass for GaAs, n is the electron density, and ϵ is the average background dielectric constant. The effective electron-electron interaction can then be written as[7]

$$V(\mathbf{r}) = \left(\frac{e^2}{\epsilon}\right) \int_0^\infty dq F(q) J_0(qr), \tag{7}$$

where

$$F(q) = \left[1 + \frac{9}{8}\frac{q}{b} + \frac{3}{8}\left(\frac{q}{b}\right)^2\right]\left(1 + \frac{q}{b}\right)^{-3}, \tag{8}$$

and J_0 is the zeroth order Bessel function. This correction softens the short range divergence of the Coulomb potential and it is well known from the study of the FQH (Ref. 7) effect that it reduces both the ground state and excitation energies. Below, we shall consider its effect also on the collective excitation energies in the multilayer systems. The electrons (or holes) on one layer interact with the electrons on the other layer via the softened Coulomb potential, but no tunneling between the layers is allowed.

Since the fundamental quantities in our formalism are the correlation and structure functions, we begin the discussion with the interlayer and intralayer correlations. The correlations in double-layer systems have recently been studied by Zheng and MacDonald (ZM) (Ref. 8) and Szymański *et al.*[9] Both groups use an approach based on the method of Singwi, Tosi, Land, and Sjölander (STLS),[10] which is also extended by Szymański *et al.* to the case of low densities. The other difference between the two methods is that Szymański *et al.* consider layers with finite thickness, whereas ZM restrict themselves to the 2D case.

As discussed below, there are some interesting differences between the results of these two calculations. In order to trace the origin of these differences, we first consider the effect of the finite thickness on the pair-correlation functions. Figure 1(a) shows the interlayer and intralayer pair-correlation functions for the electron-electron double-layer system and Fig. 1(b) the corresponding quantities for the electron-hole double-layer system, both at $r_s = 3$. The layer separation $c = 0.75$ in units $r_s a_0 = 1$, which for GaAs corresponds $c \simeq 25$ nm. The effect of the finite layer thickness is clear, although small in both cases. The finite thickness enables two similar particles to reside at the same position [at the layer coordinate $\mathbf{r} = (x, y)$], and, therefore, the intraplane pair-correlation function $g_{11}(\mathbf{r})$ is shifted from zero at the origin. This shift is, however, very small, in contrast to the result obtained by Szymański *et al.*[9] They find, for small layer separations, a very large shift of $g_{11}(0)$ both for the electron-electron and the electron-hole layer systems. This effect also increases as the density decreases, i.e., the larger the r_s, the larger the shift at the origin. In Fig. 2, we consider the effect of the density to the correlation functions for the electron-hole layer system. In this case, the layers are allowed to have finite thickness and the curves are plotted for two values of density; $r_s = 3$ and 5. The behavior of $g_{11}(0)$ is again in contrast with that in the work of Szymański *et al.*; here, the smaller the density the smaller the $g_{11}(0)$. This is the behavior familiar from both 2D (Ref. 11) and 3D (Ref. 12) electron systems. Indeed, our results are in much better agreement with those of ZM,[8] where strictly 2D electron-electron and electron-hole layer systems were considered. However, the finite thickness as such cannot be responsible for the possible compensation effect discussed by Szymański *et al.*,[9] i.e., the increase of $g_{11}(0)$, because of the formation of an attractive region to the ad-

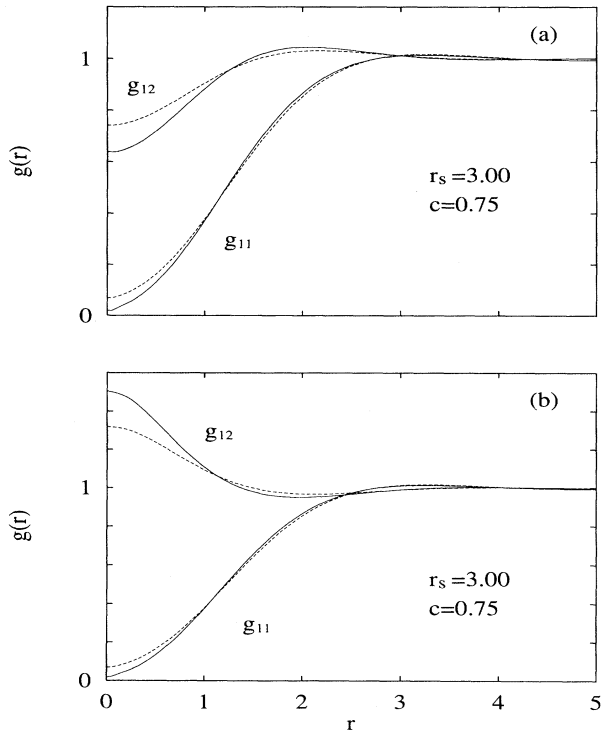

FIG. 1. The intralayer correlation functions g_{11} and interlayer correlation functions g_{12} for (a) the electron-electron and (b) the electron-hole double-layer system. The solid curves are the results for a strictly 2D calculation and the dashed curves result from the calculcation using the finite thickness correction. The layer separation $c = 0.75$ in units $r_s a_0 = 1$, where $a_0 = \epsilon\hbar^2/m_0 e^2$.

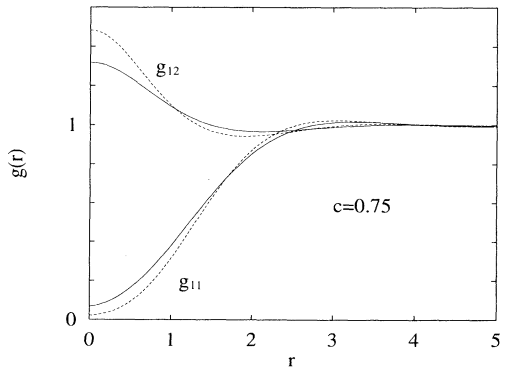

FIG. 2. The pair-correlation functions for the electron-hole double-layer system with layer separation $c = 0.75$. The density parameter $r_s = 3.0$ (solid line) and $r_s = 5.0$ (dashed line).

jacent layer. In fact, the so called "compensatory effect" might as well be an artifact of the method used in Ref. 9. Since this effect is not seen either in our calculations or in those of ZM,[8] our calculations seem to confirm the STLS result. Finally, it should be pointed out that within our scheme, the intralayer correlation function stays positive at all values of r, which is of course what is physically expected.

The collective excitations in layered electron gas systems have been studied by many authors,[13,14] usually using the random phase approximation (RPA) or the self-consistent field method. A calculation taking into account the correlations has been presented by Neilson *et al.*[15] In our scheme, the correlations are taken into account via the Jastrow wave function and the dispersion relations for the collective excitations are obtained from the extended Feynman formula.[16] In Fig. 3, we show the effect of the finite layer thickness on the excitation spectrum. It can be seen that at large values of the wave vector q, the finite thickness has the effect of depressing the curves towards smaller energy values. The lower acoustic plasmon branch and the higher optical plasmon branch tend to coincide at smaller values of q than in the case of the strictly 2D layers. Contrary to the RPA prediction,[14] which states that the acoustic plasmon is Landau damped at all densities, in our model the acoustic plasmon is degenerate with the single particle continuum only at high densities. At the experimentally relevant density region ($r_s = 2 - 5$), the acoustic plasmon is free from Landau damping. The optical branch of the excitation is always free from Landau damping.

As shown in our previous work,[5] the variational HNC method also enables the calculation of the total energy of the layer system in terms of the structure factors that are the Fourier transforms of the pair-correlation functions. From the formula for the total energy, it is straightforward to calculate the pressure and compressibility (or bulk modulus) of the system. Eisenstein *et al.*[2] showed

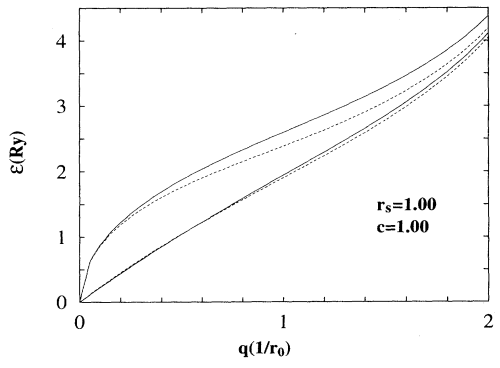

FIG. 3. The collective excitation spectra for the electron-hole layer system at $r_s = 1.0$. The layer separation $c = 1$ and the energy is in units of 1 Ry $= e^2/2\epsilon a_0$. The solid curves represent the 2D system and the dashed curves the layers with finite thickness.

TABLE I. Density parameter r_s at the zero of bulk modulus for a single electron gas layer.

Hartree-Fock	2.22
Monte Carlo[a]	2.02
Present (2D)	1.97
Present (finite thickness)	1.69
Experiment[b]	1.75

[a]Reference 11.
[b]Reference 2.

that the compressibility of a single electron gas layer reaches zero and becomes negative at a certain value of density. In Table I, we present the values of r_s where the bulk modulus goes to zero, obtained from different calculations. Our result for the 2D layer agrees well with the accurate Monte Carlo calculation of Tanatar and Ceperley.[11] In the experimental situation, the layer has naturally a finite extension in the z direction. Indeed, our result from the calculation taking into account the finite thickness of the layer agrees well with the experimental results.

As can be seen from the calculation for the single layer, the thickness of the layers causes a considerable effect to the bulk modulus. We, therefore, present results for the bulk moduli of electron-electron and electron-hole layer

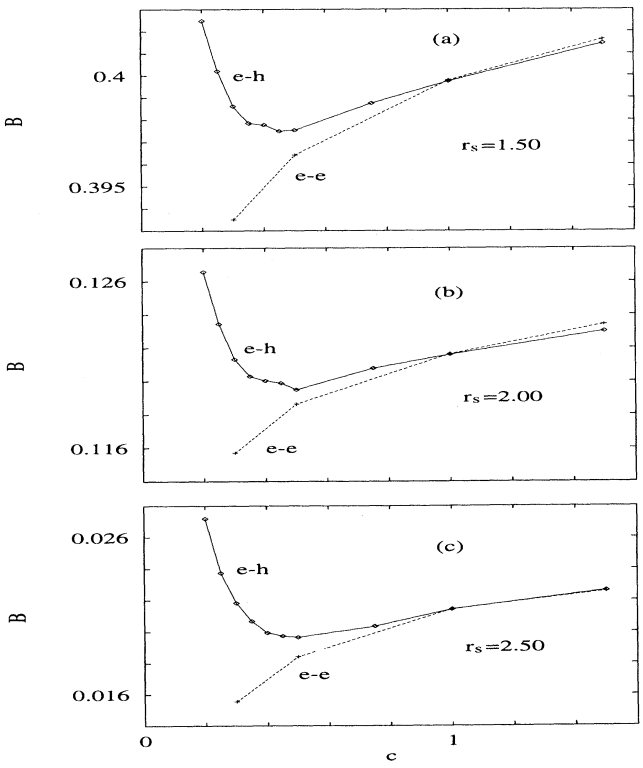

FIG. 4. Bulk modulus (in Ry/ρ^2, where ρ is the areal density of the layers) vs the interlayer separation c of the electron-hole double-layer system for (a) $r_s = 1.5$, (b) $r_s = 2.0$, and (c) $r_s = 2.5$.

systems with finite layer thickness. In Fig. 4, we show these quantities as a function of the layer separation for three different values of r_s. As discussed in an earlier paper,[5] the bulk modulus of the electron-hole system has a minimum at a certain value of the layer separation. Figure 4 shows that the shape and position of this minimum is almost density independent. We are of course dealing with a relatively narrow range of densities where, e.g., the possible charge density waves[9] do not play any role. However, also in this region there seems to exist an instability that manifests itself as the steep rise of the bulk modulus curves at small layer separations. Whether this instability is due to the exciton formation[17] or some other mechanism, cannot be concluded on the basis of our formalism. At very small layer separations, a formalism that does not take into account the tunneling between the layers, is naturally unreliable. However, at layer separations considered in Fig. 4, the tunneling should be negligible.

In conclusion, we have extended the Jastrow variational method for the calculation of the pair-correlation and structure functions in the electron-electron and electron-hole multilayer systems to the case of layers with finite thickness. The finite thickness of the layers has been shown to have a tractable effect both on the correlation functions and the dispersion relation of the collective excitations. Moreover, a quantitative agreement with experimental results of Eisenstein *et al.*[2] was obtained in the calculation for the bulk modulus of a single electron gas layer. The electron-hole layer system has a region of stability as a function of density and layer separation; at small densities, there exists a charge density wave instability[9] and at larger density, the system becomes unstable at small layer separations.

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