Energy spectrum of electrons in a parabolic quantum well in a strong magnetic field

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We study, in the $\nu=1$ quantum limit, the spin- and the charge-density excitation spectra of electrons confined in a parabolic quantum well in a strong magnetic field applied perpendicular to the electron gas. The electron-electron interaction is treated in the Hartree-Fock approximation. The inter-Landau-level dispersion relations show similar features with those calculated for a two-dimensional electron gas. On the contrary, for the intra-Landau-level charge-density excitations we found that, as the thickness of the electron layer inside the well increases, the dispersion presents a soft mode. From this we conclude that, as the two-dimensional density of electrons in the parabolic well increases, the system undergoes a phase transition, probably to a charge-density-wave state.

I. INTRODUCTION

The ability to grow selectively doped semiconductor structures has made possible the study of the properties of two-dimensional electron-gas (2DEG) systems. In particular the study of the 2DEG in presence of a strong magnetic field applied perpendicular to the electron layer has led to the discovery of the integer[1] and fractional[2] quantum Hall effects (QHE's). The integer QHE can be explained using an essentially one-electron analysis. However, the explanation of the fractional QHE is not possible in the framework of noninteracting electrons. It was needed to introduce the concept of incompressible quantum liquid in order to explain the fractional QHE.

A three-dimensional electron gas (3DEG) in presence of a strong magnetic field is also expected to show interesting and exotic properties.[3-8] Depending on the strength of the magnetic field, different kinds of broken symmetry ground states have been proposed. One can expect a spin-density-wave (SDW) ground state[3-5] at moderate magnetic fields, and a charge-density-wave (CDW) ground state[6-8] or a Wigner crystal[6-8] at high magnetic fields. Unfortunately, in the three-dimensional doped semiconductors, the interaction between the electrons and the neutralizing charged impurities is so strong that it precludes any experimental observation of any hypothetical broken-symmetry ground state in the 3DEG.[9]

In remotely doped semiconductors structures, the electrons are spatially separated from the dopant atoms, and this reduces the electron-charged impurity interaction. Thus, in order to study the properties of a 3DEG under a strong magnetic field, it seems more likely to follow the evolution of the states of a quasi-2DEG under a strong magnetic field when additional degrees of freedom, associated with the third dimension, are introduced. This third dimension has been introduced into the problem in differents ways: by means of a periodicity (superlattice) in the third dimension,[10] by fabricating a double quantum well,[11] or by growing a wide parabolic quantum well.[12]

Stormer *et al.*[10] reported measurements of the integer QHE in GaAs-$Ga_{1-x}Al_xAs$ superlattices structure when a magnetic field is applied perpendicular to the electronic layers.The electronic spectrum of this superlattice exhibits dispersion relation in the three spatial directions. In this experiment the value of the Hall conductance is interpreted[10] as $2e^2/h$ per layer. In the same kind of layered systems, and in presence of a strong magnetic field applied perpendicular to the electronic layers, MacDonald, Oji, and Bryant[13] found that, in the Hartree-Fock approximation, the electron-electron interaction favors the localization of the electronic charge in individual quantum wells and hence, the interactions drive a transition from three- to two-dimensional behavior as the electron density is increased.[13] This could explain the experimental observation of the integer QHE in superlattices.[10]

Boebinger *et al.*[11] have studied the QHE in a high-mobility double quantum well and they have observed that as the barrier thickness between the two wells increases, the plateau corresponding to the Hall resistance h/e^2 is destroyed. Calculations in the Hartree-Fock approximation[14,15] and in the single-mode approximation[16] find that the double-quantum-well system undergoes a phase transition, probably to a CDW state as the distance between the wells increases. This phase transition has been proposed[15] to be responsible for the destruction of the integer QHE in the double-quantum-well structure.[11]

The purpose of this paper is to study in the strong magnetic-field limit, the energy spectrum of a quasi-2DEG as a function of the thickness of the electron layer. In order to change the layer width we are going to use wide parabolic quantum wells (WPQW's). Remotely-doped WPQW have recently been proposed[4,17] as a system where the transition between high-mobility quasi-2DEG and quasi-3DEG can be realized. Poisson's equation implies that a parabolic potential $V_0(z)=Az^2$ is equivalent to the potential created by a uniform slab of positive charge of three-dimensional density n_0 =

$A\epsilon/2\pi e^2$, where e is the electron charge and ϵ is the dielectric constant of the system. Electrons, which arise from donor impurities located away from the well, enter the well and screen this *fictitious* background, forming a uniform layer of thickness n_S/n_0, where n_S is the two-dimensional density of electrons in the system. In this way it is possible to design heterostructures where a thick (>2000 Å) slab of electrons exists in practice.

Those WPQW's have recently been grown[12] by changing quadratically the aluminum concentration in a $Al_xGa_{1-x}As$ heterostructure. Magneto-optical experiments[18] have shown[19] that the system holds a uniform slab of high-mobility electron gas. Both the integer[12] and fractional[20] QHE have been observed in WPQW's. Shayegan *et al.*[20] found that in the WPQW's the fractional QHE collapses as the thickness of the electron layer increases. This effect was explained theoretically by He *et al.*[21] as an effect of weakening of the short-range component of the electron-electron interaction. In addition, the WPQW system in the presence of a moderate magnetic field applied parallel to the electron slab, has been proposed as a system where a SDW instability, characteristic of a 3DEG,[3] can occur.[22]

In this paper we restrict our study to the calculation of the electronic properties of a WPQW system in the presence of a strong magnetic field, applied perpendicular to the electron slab and corresponding to the filling factor ν=1. We are going to treat the electrons in the Hartree-Fock (HF) approximation. First, we calculate self-consistently the eigenstates and eigenvalues of the *normal* state of the system and from this, the excitation spectrum. By *normal* state we mean a uniform distribution of the electron charge in the plane perpendicular to the growth direction.

The excitation spectrum of this system is obtained from the poles of the response functions of the system. To find the response functions we use the self-consistent approximation discussed by Kallin and Halperin[23] and independently by MacDonald.[24] The poles of the spin-density response function give the energies of the spin-density excitations (SDE's) and the poles of the charge density response function those of the charge-density excitations (CDE's). In this framework, the existence of soft modes indicates that the system undergoes a phase transition.

This paper is organized as follows. In Sec. II we describe the approximation we use in order to obtain the energies and wave functions of the *normal* state of the WPQW. In Sec. III we introduce the formalism used in order to obtain the CDE and the SDE spectra. Section IV is dedicated to show our results, and we conclude with a summary in Sec. V.

II. ENERGIES AND WAVE FUNCTIONS

In this section we calculate self-consistently in the HF approximation the self-energies and wave functions of the *normal* state of the WPQW.

The electrons are treated in the effective-mass approximation, they are characterized by an effective mass m^* and an effective Landé factor g^*. These parameters, g^* and m^*, take the band effects of the host semiconductor into account. We do not include in our calculations the variations of the effective mass and the effective Landé factor across the well. Also we take the dielectric function of the host semiconductor as constant. In the actual WPQW's,[12,18,20] these quantities have only a small variation from the center to the edge of the well and including this variation in the calculation does not produce qualitative changes in our results.[25] Also omitted from the calculation are the nonparabolicity of the conduction band and the band-mixing effects induced by confinement. We take the z direction as the growth direction and assume translational invariance in the x-y plane as a consequence of our effective mass approach. The magnetic field is applied in the z direction and we choose the Landau gauge, $\mathbf{A}=(0, Bx, 0)$. Under these conditions and using the fact that in the *normal* state the (x, y) part of the single wave function is the same in the HF approximation as in the case of independent electrons,[3] the energies and wave functions of the *normal* state in the HF approximation take the form

$$\psi_{n,i,k_y,s_z}(\mathbf{r}) = \frac{1}{\sqrt{L}} e^{ik_y y} \varphi_n(x - k_y \ell^2) \phi^n_{i,s_z}(z)|s_z\rangle, \quad (1)$$

$$\varepsilon_{n,i,s_z} = (n + \tfrac{1}{2})\hbar\omega_c + E^n_{i,s_z}. \quad (2)$$

Here L is the linear sample dimension, φ_n are the orthonormal eigenstates of the one-dimensional harmonic oscillator, s_z is the z component of the electron-spin variable[26] ($\pm\frac{1}{2}$), $|s_z\rangle$ is the spin-wave function, $\omega_c = eB/m^*c$ is the cyclotron frequency, and $\ell = \sqrt{\hbar c/eB}$ is the magnetic length. The energies do not depend on k_y, and therefore there is a degeneracy $L^2/2\pi\ell^2$ of each level which is associated with the different possibilities of locating the center of the one-dimensional harmonic oscillator. In Eqs. (1) and (2) ϕ^n_{i,s_z} and E^n_{i,s_z} are the orthogonal solutions of

$$[-g^*\mu_B B s_z + V_0(z) + V_H(z)]\,\phi^n_{i,s_z}(z) - \sum_{n',i',\mathbf{q}} \bar{\nu}(n', i', s_z) S_{n,n'}(q) \times \int dz_1 V(q, |z - z_1|) \phi^{n'}_{i',s_z}(z_1)\, \phi^n_{i,s_z}(z_1)\, \phi^{n'}_{i',s_z}(z) = E^n_{i,s_z} \phi^n_{i,s_z}(z). \quad (3)$$

In this expression μ_B is the Bohr magneton, $V_0(z)$ is the man-made potential, $V_H(z)$ is the Hartree potential, $\mathbf{q}$ is a two-dimensional wave vector in the x-y plane, $S_{n,n'}$ is given by the following expression,

$$S_{n,n'}(q) = \left| \int dx\, e^{iqx}\, \varphi_n(x)\, \varphi_{n'}(x) \right|^2, \quad (4)$$

and $V(q, |z|)$ is the Fourier transform, in the x-y plane,

of the interaction potential between the electrons. In our case the electrons interact by means of a Coulomb potential screened by the dielectric constant of the host semiconductor, so that

$$V(q,|z|) = \frac{2\pi e^2}{\epsilon}\frac{e^{-q|z|}}{q} \quad . \tag{5}$$

In Eq. (3) $\bar{\nu}(n,i,s_z)$ is the filling factor of the state characterized by the quantum numbers (n,i,s_z); these coefficients are chosen so that they verify the following conditions: (i) the maximum value of $\bar{\nu}$ is unity, (ii)

$$n_S = \frac{1}{2\pi\ell^2}\sum_{n,i,s_z}\bar{\nu}(n,i,s_z) \quad , \tag{6}$$

and (iii) the total HF energy of the system

$$E_T = \frac{1}{4\pi\ell^2}\sum_{n,i,s_z}\bar{\nu}(n,i,s_z)\left(\varepsilon_{n,i,s_z} + \int |\phi^n_{i,s_z}(z)|^2 V_0(z)dz - g^*\mu_B B s_z\right), \tag{7}$$

is minimized. The filling factor of the system ν is equal to the sum of the filling factors $\bar{\nu}$ of the states.

The Hartree term due to the electrostatic interaction of the electrons with themselves and with the impurity charges is obtained from

$$\frac{d^2V_H(z)}{dz^2} = -\frac{4\pi e^2}{\epsilon}[n(z) - N_D(z)] \quad , \tag{8}$$

where $N_D(z)$ is the actual density of positive charge, located away from the well, necessary to mantain charge neutrality, and $n(z)$ is the electron density

$$n(z) = \frac{1}{2\pi\ell^2}\sum_{n,i,s_z}\bar{\nu}(n,i,s_z)\,|\phi^n_{i,s_z}(z)|^2. \tag{9}$$

In Eq. (3) the last term of the left side corresponds to the exchange self-energy, and $V_H(z)$ corresponds to the direct term of the self-energy. In Fig. 1(a), the diagrammatic representation of the self-energy corrections in the HF approximation is shown. In the case of wide quantum wells it is very important to take into account the direct term of the self-energies; for WPQW's this term is responsible for the existence of a thick slab of electron gas.[27,28]

The calculation process consists of finding the filling factor $\bar{\nu}(n,i,s_z)$ which minimizes the total energy, Eq. (7) of the system, and then obtaining the energies and wave functions. We remark here, that besides the HF and the effective-mass approximations, another extra assumption we use in Eqs. (1)–(9) is that the charge and the spin are uniformly distributed in the x-y plane, in other words that the system is in the *normal* state.

III. RESPONSE FUNCTIONS AND COLLECTIVE EXCITATIONS

In this section we describe the formalism we use in order to obtain the response function and the excitation

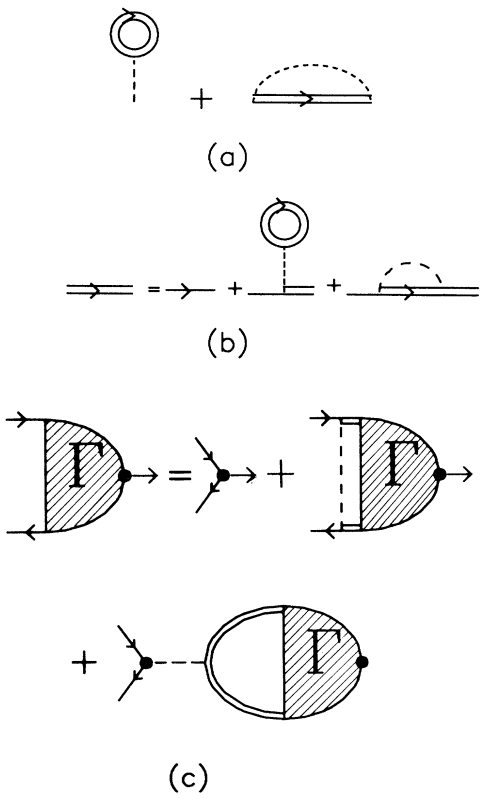

FIG. 1. Diagrammatic representation of the approximation used in this work for the calculation of (a) the self-energy and (c) the vertex function. In (b) we show the scheme of the single-particle Green's function.

modes of the system in the presence of a strong magnetic field applied perpendicular at the electronic slab. The poles of the response functions represent neutral excitations of the system.

The charge-density response function has the form

$$\chi_\rho(z,z',\mathbf{q},\omega) = -i\int_0^\infty dt\, e^{i\omega t}\langle[\rho(\mathbf{q},z',t),\rho^+(\mathbf{q},z,0)]\rangle, \tag{10}$$

where $\langle\rangle$ denotes quantum-mechanical and thermal averaging and $\rho(\mathbf{q},z,t)$ is the Heisenberg representation of the density operator

$$\sum_{i=1}^{N} e^{i\mathbf{q}\mathbf{r}_i}\,\delta(z_i) \quad ,$$

where $\mathbf{r_i} = (x_i,y_i,z_i)$ is the position operator of the ith electron and N is the total number of electrons in the system.

In the same form the spin-density response functions are

$$\chi_{\sigma_\pm}(z,z',\mathbf{q},\omega) = -i\int_0^\infty dt\, e^{i\omega t}\langle[\sigma_\pm(\mathbf{q},z',t),\sigma_\pm^\dagger(\mathbf{q},z,0)]\rangle \tag{11}$$

and

$$\chi_{\sigma_z}(z,z',\mathbf{q},\omega) = -i\int_0^\infty dt\, e^{i\omega t}\langle[\sigma_z(\mathbf{q},z',t),\sigma_z^\dagger(\mathbf{q},z,0)]\rangle, \tag{12}$$

where $\sigma_\pm \equiv (\sigma_x \pm i\sigma_y)/\sqrt{2}$ and $\boldsymbol{\sigma}(\mathbf{q},z,t) \equiv (\sigma_x,\sigma_y,\sigma_z)$ are the Heisenberg representation of the spin operators

$$2\sum_{i=1}^{N} e^{i\mathbf{q}\mathbf{r}_i}\delta(z_i)\mathbf{S}_i,$$

where $\mathbf{S}_i$ is the spin angular momentum operator for the ith electron.

Assuming that the system is in the *normal* state, the response functions only depend on the modulus of $\mathbf{q}$, and the charge-density and spin-density response functions can be written in terms of the vertex functions Γ^ρ and Γ^σ as

$$\chi_A(z,z',q,\omega) = \frac{1}{2\pi\ell^2}\sum_\alpha\sum_{\alpha'}\phi^n_{i,s_z}(z)\,\phi^{n'}_{i',s'_z}(z)F_{n',n}(0,q)\langle s'_z|\Theta_A|s_z\rangle\frac{f(\varepsilon_\alpha)-f(\varepsilon_{\alpha'})}{\varepsilon_\alpha-\varepsilon_{\alpha'}+\hbar\omega}\,\Gamma^A_{\alpha',\alpha}(z',q,\omega)\ , \tag{13}$$

where $A=\rho$, σ_z, or $\sigma_\pm$ and $\Theta_\rho=1$, $\Theta_{\sigma_z}=2S_z$, and $\Theta_{\sigma_\pm}=2S_\pm$, f is the Fermi distribution function and the label α stands for the Landau level n, the band index i, and the spin index s_z, e.g., $\alpha \equiv (n,i,s_z)$. The function $F_{n,n'}$ is defined as

$$F_{n',n}(\mathbf{q}) \equiv \frac{n!}{n'!}\left(\frac{(-q_y+iq_x)\ell}{\sqrt{2}}\right)^{n'-n}\exp\left(\frac{-q^2\ell^2}{4}\right)L_n^{n'-n}\left(\frac{q^2\ell^2}{2}\right), \tag{14}$$

for $n' \geq n$, and for $n' < n$ is obtained using the identity $F_{n,n'}(\mathbf{q}) = F^*_{n',n}(-\mathbf{q})$. In the last equation $L_n^\alpha(x)$ is a generalized Laguerre polynomial.

We treat the response function in the framework of the self-consistent HF approximation as we did before in the calculation of the self-energies. We keep only the terms which correspond to a single exciton present at all times, neglecting terms with two or more excitons present. With this rule, in the self-consistent HF approximation, the vertex part of Eq. (13) satisfies the following integral equation:

$$\begin{aligned}\Gamma^A_{\alpha',\alpha}(z',q,\omega) = {} & F_{n',n}(0,q)\,\phi^n_{i,s_z}(z')\,\phi^{n'}_{i',s'_z}(z')\langle s_z|\Theta_A^\dagger|s'_z\rangle \\ & - \sum_{\alpha'',\alpha'''}\Gamma^A_{\alpha''',\alpha''}(z',q,\omega)\frac{f(\varepsilon_{\alpha'''})-f(\varepsilon_{\alpha''})}{\varepsilon_{\alpha'''}-\varepsilon_{\alpha''}+\hbar\omega}\left[g_{\alpha,\alpha''',\alpha',\alpha''}(q)-v_{\alpha,\alpha''',\alpha'',\alpha'}(q)\right],\end{aligned} \tag{15}$$

where

$$\begin{aligned}g_{\alpha,\alpha''',\alpha',\alpha''}(q) = {} & \delta_{s_z,s''_z}\delta_{s'_z,s'''_z}\sum_{\mathbf{q}'}e^{-iq'_x\ell^2q}\frac{2\pi e^2}{\epsilon q'}F_{n'',n}(\mathbf{q}')F_{n',n'''}(-\mathbf{q}') \\ & \times\int dz_1\int dz_2\, e^{-q'|z_1-z_2|}\phi^n_{i,s_z}(z_1)\phi^{n''}_{i'',s_z}(z_1)\phi^{n'}_{i',s'_z}(z_2)\phi^{n'''}_{i''',s'_z}(z_2)\end{aligned} \tag{16}$$

and

$$\begin{aligned}v_{\alpha,\alpha''',\alpha'',\alpha'}(q) = {} & \delta_{s_z,s'_z}\,\delta_{s''_z,s'''_z}\frac{e^2}{\epsilon\ell^2 q}F_{n',n}(0,-q)F_{n'',n'''}(0,q) \\ & \times\int dz_1\int dz_2 e^{-q|z_1-z_2|}\,\phi^n_{i,s_z}(z_1)\phi^{n'}_{i'',s_z}(z_1)\phi^{n''}_{i''',s''_z}(z_2)\phi^{n'''}_{i''',s''_z}(z_2).\end{aligned} \tag{17}$$

The diagrammatic representation of the vertex function Γ^A is given in Fig. 1(c). The term in the vertex function proportional to $v_{\alpha,\alpha''',\alpha',\alpha''}$ [last term in Fig. 1(c)] represents processes where the electron and the hole annihilate each other at one point in space and one electron-hole pair is created simultaneously at another point. The term proportional to $g_{\alpha,\alpha''',\alpha'',\alpha'}$ [second term in Fig. 1(c)] describes the Coulomb interaction of the excited electron and hole. This term is neglected in the random-phase approximation (RPA), which only includes terms proportional to $v_{\alpha,\alpha''',\alpha',\alpha''}$.

We should mention here that the HF approximation neglects any kind of screening of the Coulomb interaction by the electron gas. This approximation is exact to first order in the expansion parameter, which typically is the interaction energy divided by the minimun energy gap. In the work of Kallin and Halperin,[23] in a 2D system in the strong magnetic-field limit, the expansion parameter was small and the use of the HF approximation was justified. In WPQW's and for integer values of ν, the gap

energy is comparable to the interaction energy and we are less confident in using this approximation. A higher-order approximation is quite difficult and most probably would give qualitatively similar results. Then we keep working in the HF approximation.

The dispersion relations of the collective excitations of the system, $\omega(q)$, are obtained from the poles of the response functions which, as seen in Eq. (13), coincide with those of the vertex functions and, as deduced from Eq. (15), correspond to the eigenvalues of the matrix

$$(\varepsilon_{\alpha'}-\varepsilon_{\alpha})\delta_{\alpha''',\alpha'}\delta_{\alpha'',\alpha}+[f(\varepsilon_{\alpha'''})-f(\varepsilon_{\alpha''})] \times[g_{\alpha,\alpha''',\alpha',\alpha''}(q)-v_{\alpha,\alpha''',\alpha'',\alpha'}(q)]. \quad (18)$$

The character of each excitation, spin, or charge density, can be obtained from the structure of the corresponding eigenvector. From Eq. (18) we see that the excitation energies of the system are shifted from the difference in energies of the electron and the hole by the Coulomb binding energy (g term) and by a RPA energy (v term). This RPA term does not appear in the SDE's, where the electron and the hole have different z component of the spin. It is not possible for an electron-hole pair with antiparallel spins to recombine through the Coulomb potential, in a RPA-like process as those which appear in the CDE's.

Due to the magnetic field,[23] the expected value of the difference vector position of the electron and the hole of an exciton of wave vector $\mathbf{q}$ is $\ell^2\mathbf{q}\times\hat{\mathbf{z}}$, where $\hat{\mathbf{z}}$ is a unitary vector in the z direction. Then, an exciton with a very large q coresponds to a pair where the electron and the hole are separated by a large distance, so that the electron-hole interaction is very small. Thus the exciton energy in the $q\rightarrow\infty$ limit should be equal to the difference between the energies of the independent electron and hole.

The consistency of the HF approximation we are using can be checked by looking at some long-wavelength excitation energies. Independently of the shape of the man-made potential $V_0(z)$, and of the number of electrons in the system, we should verify Kohn's theorem,[29] that when the wave vector of the exciton is zero, there is a CDE with energy exactly equal to $\hbar\omega_C$. Also we should get, in agreement with Larmor's theorem, that, in $q=0$, the lowest SDE energy is $|g^*\mu_B B|$. When the confining potential has a parabolic form, we also should obtain that, at $q=0$, the energy of one of the CDE's has the value $\hbar\omega_0$, where ω_0 is the bare harmonic-oscillator frequency of the quadratic potential.[19]

IV. RESULTS

In this section we are going to show our results for the case of a parabolic potential and in the strong magnetic field limit $\nu=1$. The parabolic potential is characterized by a bare harmonic-oscillator frequency ω_0,

$$V_0(z)=\tfrac{1}{2}m^*\omega_0^2 z^2 \ . \quad (19)$$

As mentioned above, classically the electrons trapped in the well distribute themselves in a uniform layer of density

$$n_0=\frac{\omega_0^2 m^*\epsilon}{4\pi e^2} \quad (20)$$

and thickness n_S/n_0.

In order to describe the experimentally used $Ga_{1-x}Al_xAs$ WPQW's we take $m^*=0.067$, $\epsilon=12.5$, and $g^*=0.44$. In our calculations the background of positive charge, $N_D(z)$, consists of two layers of equal density, 200 Å thick and located symmetrically 2200 Å from the center of the well. We have checked that, for reasonable choices of the parameters, our results are insensitive to the precise location of the positive charges. All the calculations, unless we say otherwise, have been performed for a parabolic potential characterized by an energy $\hbar\omega_0=2.92$ meV. This value of ω_0 describes the curvature of some WPQW samples.[12] Regarding the magnetic field, it is varied when changing n_S so that all the results correspond to the $\nu=1$ quantum limit ($B=2\pi n_S\hbar c/e$).

A. Energies and wave functions

In the $\nu=1$ quantum limit, $\bar{\nu}(\alpha)=0$ for all α, except for the lowest-energy state. From the calculation of the HF total energy, Eq. (7), we have checked that in this limit the ground state is spin polarized and the occupied state corresponds to the quantum numbers (0,1,+). In the following we are going to denote the value of the z component of the spin by $\pm$, corresponding to the values $\pm\frac{1}{2}$.

In Fig. 2, the variation of the energies ε_{n,i,s_z} as a function of the two-dimensional density of electrons in the system n_S is shown. In Fig. 2(a), we show the energies corresponding to states with the same spin as the occupied state, and in Fig. 2(b) the energies corresponding to states with spin flipped with respect to the spin of the occupied state. As commented at the end of the previous section, the differences of energies shown in Fig. 2 correspond to the energy of a exciton where the electron and the hole are infinitely separated and they cannot interact, that is, to the long-wave-vector limit of the collective excitations of the system. Then, the lowest gap in Fig. 2 is responsible for the plateau $\nu=1$ in the QHE.

From Fig. 2 we see that in a parabolic potential with $\hbar\omega_0=2.92$ meV and for densities corresponding to electron layers wider than 700 Å, the lowest gap energy corresponds to transitions where the spin is not flipped. The lowest energy transition always corresponds to an intra-Landau-level excitation. Note that due to the exchange self-energy, the smallest gap in the HF approximation is much larger than would be obtained in the Hartree approximation.[27] Since this gap is responsible for the plateau $\nu=1$ in the QHE, we conclude that in the *normal* state, even for very large electron thickness, it is possible to observe this plateau in the transverse magnetoresistence.

From Fig. 2 we observe that except for very low densities the energy separation decreases with increasing n_S. This reduction is due to two reasons.

(1) The thickness of the uniform slab of electrons, which is formed inside the parabolic well, increases linearly with n_S, thus the effective confinement[27] due to

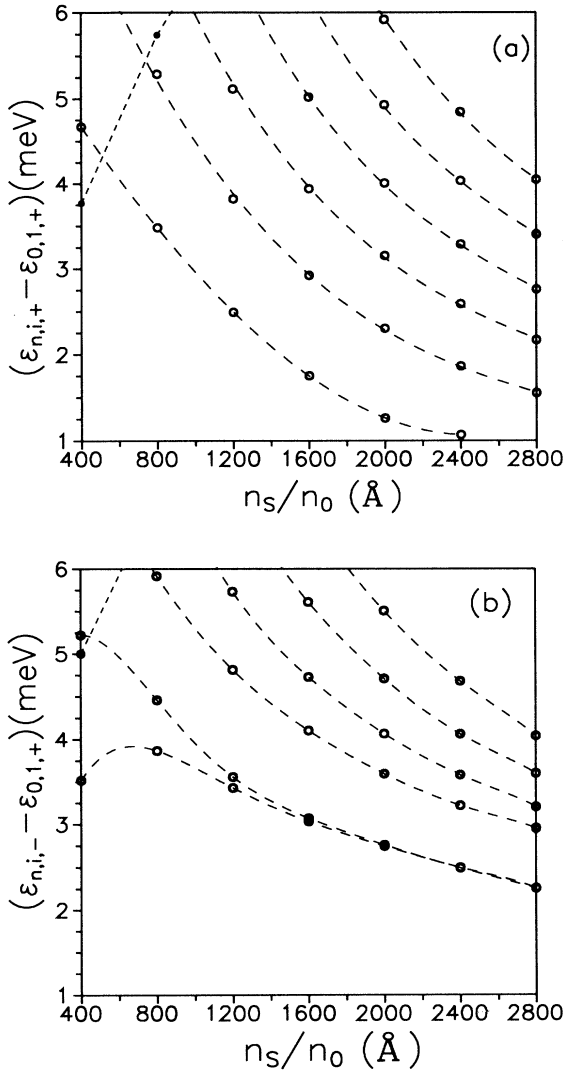

FIG. 2. Variation as a function of the effective electron thickness of the energy of the states (a) with spin parallel to the magnetic field and (b) with spin antiparallel to the magnetic field. The parabolic potential has a curvature $\hbar\omega_0$=2.92 meV and the filling factor is 1. The closed circles show the states corresponding to the second Landau level. The other parameters used in the calculation are given in the text.

the sum of the initial potential and the Hartree potential decreases with increasing n_S.

(2) Since the value of ν is fixed to 1, the variation of n_S implies the variation of the magnetic field and exchange effects decrease when B increases.

The different behavior of the energy separation $\varepsilon_{n,i,-} - \varepsilon_{0,1,+}$ at very low densities occurs because in this range of n_s the increase of the exchange effects due to the increase of the number of electrons in the system is more important than the reduction of the exchange effects due to the increase of the magnetic field.

In Fig. 3 we plot the wave functions corresponding to

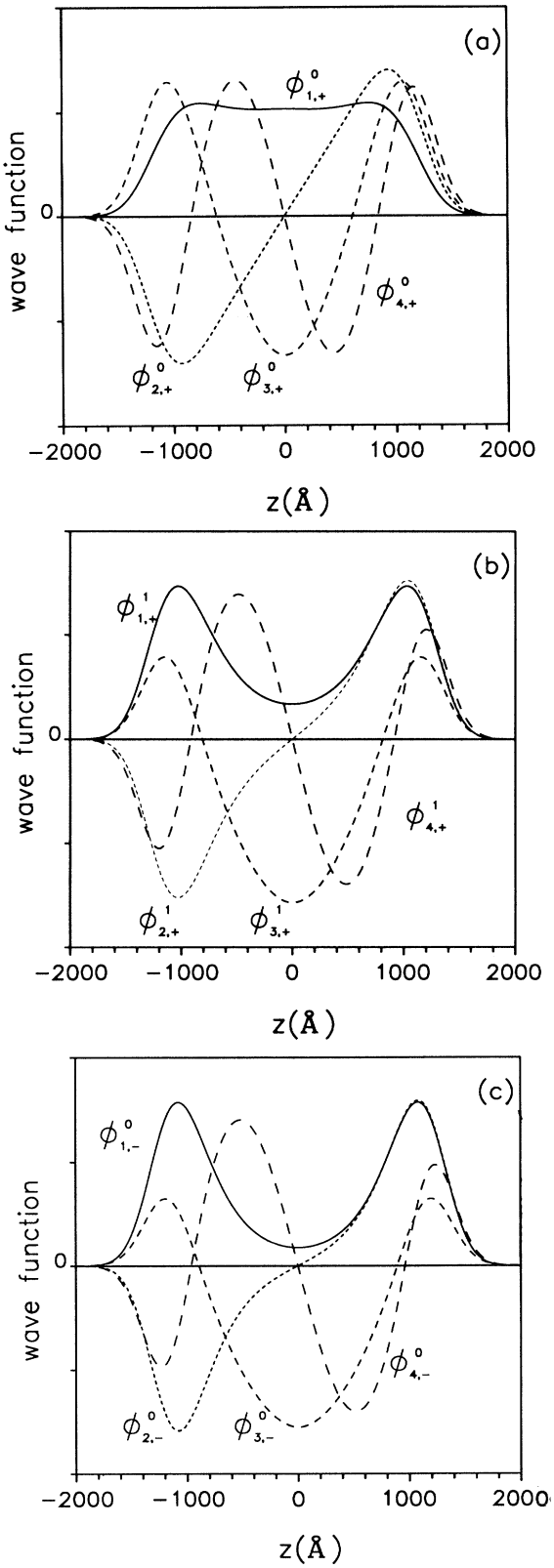

FIG. 3. Self-consistent wave functions for a parabolic potential with $\hbar\omega_0$=2.92 meV and a 2D density of electron n_s/n_0=2400 Å, in the ν=1 quantum limit. The other parameters used in the calculation are given in the text.

the lowest energies of our system for a value of n_s/n_0 equal to 2400 Å. Since we are working in the $\nu=1$ case, the wave function of the lowest state has the form of the square root of the charge-density profile of the system. Then from the shape of $\phi^0_{1,+}$ in Fig. 3(a), we know that in the system exists a thick and rather uniform slab of electronic charge. The main difference between the charge-density profiles, with and without a magnetic field,[27] is that the magnetic field smooths the small bumps which appear without magnetic field at the edge of the electronic slab.[27,28] This is because with $\nu=1$ the system has only one state occupied.

In Figs. 3(b) and 3(c) are shown the wave functions corresponding to the second Landau level with the spin parallel to the magnetic field, $\phi^1_{i,+}$, and those corresponding to the first Landau level with the spin antiparallel to the magnetic field, $\phi^0_{i,-}$. Note that in both cases the lowest states, $\phi^1_{1,+}$ and $\phi^0_{0,-}$, have more weight at the edges of the electronic slab than in the center. This reduces the separation in energy between the states (1,2,+) and (1,1,+) and between the states (0,2,−) and (0,1,−). This effect can be also observed in Fig. 2(b), where the state (0,2,−) becomes degenerate at high densities with the (0,1,−). The reason for this behavior can be understood in the following way. Since the exchange interaction has an attractive effect, in order to create in the center of the well an almost flat effective potential for the occupied state and a uniform distribution of electrons inside the well, the sum of the man-made potential and the self-consistent Hartree potential should cancel the shape of the self-consistent exchange potential. Then the sum $V_0(z)+V_H(z)$ acquires a concave form in the center of the well and has a minimum at each edge of the electronic slab. Since the ground state is spin polarized, the electrons with spin antiparallel to the magnetic field are not affected by the exchange term of Eq. (3) and they only feel the potentials $V_0(z)$ and $V_H(z)$. Then the wave functions of electrons with spin antiparallel to B are localized at the edges of the electronic slab. These wave functions, localized at the edges of the electronic slab, become more separated as the thickness of the electron gas increases. Then, the interaction between such wave functions becomes weaker. In this form the states (0,2,−) and (0,1,−) become closer in energy as n_S increases. Something similar happens to the (1,1,+) and (1,2,+) states, in this case the energies of these states have an exchange self-energy term, but this contribution is much smaller than the exchange correction to the energy of the lowest Landau level. In other words, in Eq. (3), $S_{1,0}(q)$ is much weaker than $S_{0,0}(q)$.

B. Collective excitations

Once we know the energies and wave functions of the system, we have the necessary ingredients for obtaining the dispersion relations of the collective excitations. In the $\nu=1$ quantum limit the matrix to diagonalize in order to obtain the dispersion relations, Eq. (18), simplifies considerably. It consists of independent blocks, each of them describing one kind of excitation of the system. Since in the $\nu=1$ limit only one spin state of the lowest state is occupied, the two possible kinds of excitations are the following.

(i) CDE's corresponding to the poles of χ_ρ. In these excitations the electron and the hole have the same spin orientation. We denote the frequency of these excitations by $\omega^C(q)$. In this quantum limit, the poles of χ_{σ_z} coincide with the poles of χ_ρ.

(ii) SDE's corresponding to the poles of χ_{σ_-}. In these excitations the electron and the hole have different spin orientation. We denote the frequency of these excitations by $\omega^S(q)$. Since in this quantum limit the ground state is spin-up polarized, χ_{σ_+} does not have poles at positive frequencies.

In Fig. 4(a) we show the variation of the energies corresponding to the $q=0$ CDE's of our system as a function of the 2D density of electrons. Note that due to the quadratic form of the confining potential, one of the $q=0$ CDE's always has the value $\hbar\omega_0$.[19] Also in Fig. 4(a) it

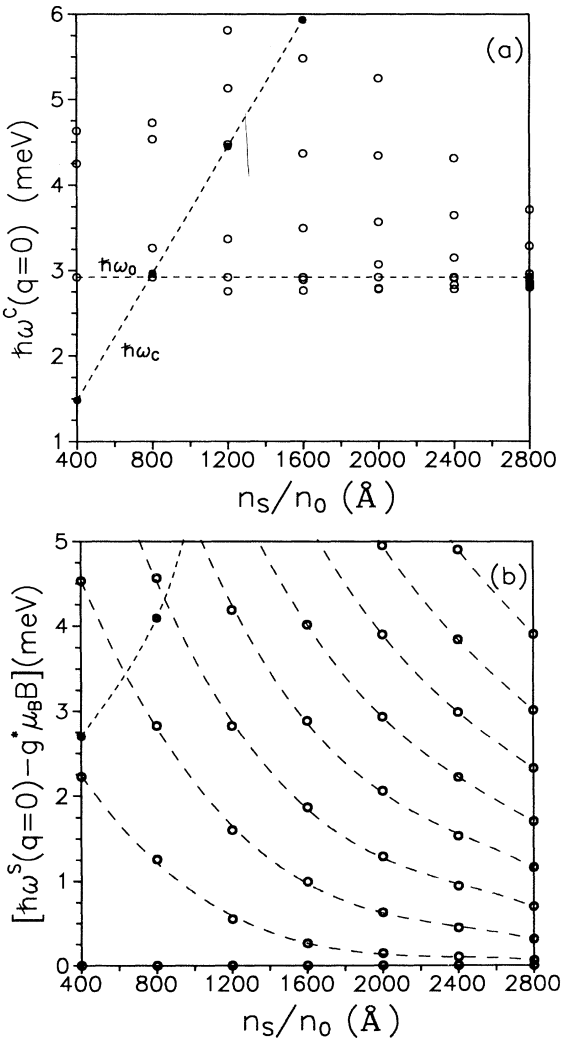

FIG. 4. Variation as a function of the effective electron thickness of the $q=0$ (a) CDE's and (b) SDE's of a parabolic well with $\hbar\omega_0=2.92$ meV and in the $\nu=1$ quantum limit. The closed circles show inter-Landau-level transitions. In (a) the dashed lines correspond to the energies $\hbar\omega_0$ and $\hbar\omega_C$. The other parameters used in the calculation are given in the text.

is showed that, as required by Kohn's theorem,[29] in $q=0$ exists an exact cancellation between the exchange enhancement of the first inter-Landau-level transition and the vertex correction to the energy excitation. It has been shown,[19] that ω_0 and ω_C are the only frequencies at which the system absorbs long-wavelength light, at $q=0$ the dipole matrix element can only connect the ground state with excitations of frequency ω_0 or ω_C. Apart from the two straight lines [dashed lines in Fig. 4(a)] corresponding to ω_0 and ω_C, the other excitations at $q=0$ show a rather complicated dependence on n_S.

In Fig. 4(b), the energy variation of the $q=0$ SDE's as a function of the effective thickness of the electron layer is shown. This figure shows that as required by Larmor's theorem[23] the lowest-energy SDE has the value $g^*\mu_B B$, independently of the number of electrons in the system. Since the exchange interaction decreases with the magnetic field, the energies of the intra-Landau-level SDE's decrease with n_S. For the same reason the energies corresponding to inter-Landau-level transitions increase slower than $\hbar\omega_C$. Note from Fig. 4, that for all the values of n_S the energies corrresponding to the SDE's are lower in energy than those corresponding to the CDE's.

In Fig. 5 we show the wave-vector dependence of the energy of the SDE's of the case $n_S/n_0=1200$ Å. The dashed lines correspond to the SDE's having an inter-Landau-level character at $q=0$. Only in $q=0$ the inter- and intra-Landau-level excitations are extrictly decoupled, but the mixing is small for $q \neq 0$. For $q\ell \ll 1$ the energy spectrum of the inter-Landau-level SDE's varies quadratically with $q\ell$. This behavior is the same for differents n_S and it is of the form one expects for spin-flip excitations.[23] The energy spectrum of the intra-Landau-level SDE's, dashed lines in Fig. 5, is practically independent of the wave vector when $q\ell \ll 1$. For thiner electron slab the dispersion relations corresponding to intra-Landau-level SDE's show a weak minimum at $q\ell \sim 1$. This behavior is similar to that obtained by Kallin[30] for the variation of the dispersion relation of this excitation in a 2DEG when the finite thickness of the electron wave function is included in the calculation.

In Fig. 6 are shown the CDE dispersion relations of our system in the case $n_S/n_0=920$ Å. The inter-Landau-level transitions, dashed lines, show the same features as the ones obtained by Kallin and Halperin[23] for the lowest magnetoplasmon of a 2DEG with $\nu=1$. The lowest inter-Landau-level excitation dispersion curve has a maximun at $q\ell \sim 0.65$ and a minimum at $q\ell \sim 1.9$. When the number of electrons in the system increases, the minimum and maximum become smoother, in a way similar to which the lowest-energy magnetoplasmon dispersion of a 2DEG with $\nu=1$ changes when the finite thickness of the electron wave function is included.[30] More interesting is the behavior of the dispersion relation corresponding to the lowest intra-Landau-level transitions (continuous lines in Fig. 6). For $q\ell < 1$ the dispersion relation decreases with the wave vector, developing a minimum at values $q\ell \sim 1.5$. When the thickness of the electron gas increases (n_S increases) this minimun becomes deeper and for a concentration of electrons higher than a critical value the dip becomes a soft mode which indicates that the system undergoes a phase transition. For a parabolic well with $\hbar\omega_0=2.92$ meV, we found that the critical thickness of the electron gas is $d^C \sim 930$ Å.

The fact that for a critical 2D density of electrons in the system and for a critical wave vector the energy of a CDE becomes zero implies that the static charge-density response function of the system diverges at this wave vec-

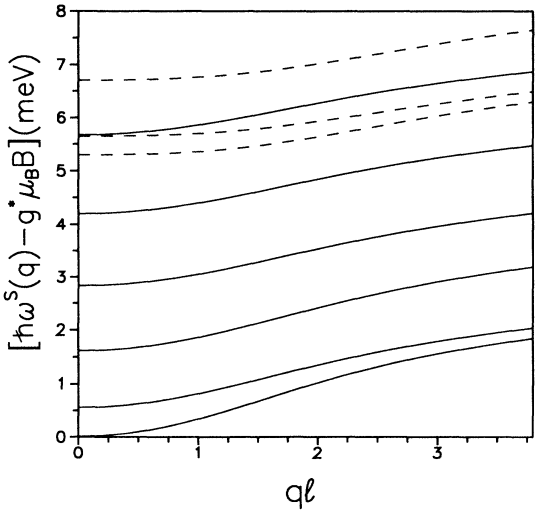

FIG. 5. Dispersion relation of the SDE's for a parabolic potential with $\hbar\omega_0=2.92$ meV, a 2D density of electrons $n_s/n_0=1200$ Å, and in the $\nu=1$ quantum limit. The dashed lines correspond to excitations which in $q=0$ have an inter-Landau-level character. The other parameters used in the calculation are given in the text.

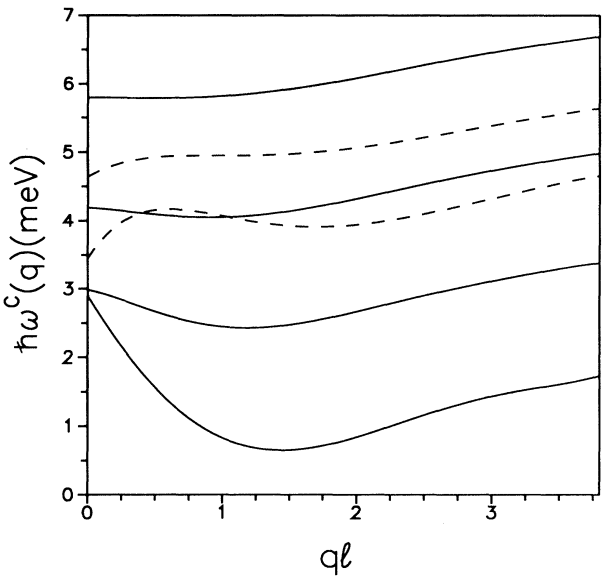

FIG. 6. Dispersion relation of the CDE's for a parabolic potential with $\hbar\omega_0=2.92$ meV, a 2D density of electrons $n_s/n_0=920$ Å, and in the $\nu=1$ quantum limit. The dashed lines correspond to excitations which in $q=0$ have an inter-Landau-level character. The other parameters used in the calculation are given in the text.

tor. Then we expect that the phase transition we have found leads the system to some kind of charge-density-wave ground state. Since the dispersion relations $\omega^C(q)$ do not depend on the direction of the wave vector q, we expect some crystallization of the electron gas in the x-y plane. Since the soft-mode excitations are mixing the lowest with higher states, the CDW phase should have a far from homogeneous shape in the z direction.

In Fig. 7 we show the variation of the critical thickness, d^C, where the minimum of the dispersion relation of the CDE's goes to zero, as a function of the curvature of the well, ω_0. Note that the change in the curvature of the well also implies a change in the designed 3D density of electrons n_0. Then in Fig. 7 we also show the corresponding values of the density parameter

$$r_S^* = \frac{m^* e^2}{\epsilon \hbar^2} \left(\frac{3}{4\pi n_0} \right)^{1/3} .$$

According to the argument that the occurrence of a soft mode in $\omega^C(q)$ implies that the system undergoes a phase transition to a CDW ground state, we can see Fig. 7 as the phase diagram of the system, the shaded part corresponding to the region where the electron gas has crystallized.

From Fig. 7 we conclude that independently of the curvature of the parabolic potential, for a sufficiently thick slab of electrons, the system undergoes a phase transition. The final nature of the new state cannot be inferred from our calculation. However, we have obtained some features that, in combination with other theoretical works,[13,31] give us some clues about the nature of the new state. In Ref. 31 MacDonald and Bryant studied, in the unrestricted HF approximation, a 3DEG in the presence of a strong magnetic field; they found that in this system the electrons not only crystallize in the direction parallel to the magnetic field, but also in the plane perpendicular to it. The electron gas forms charged rods oriented parallel to the field as proposed by Kaplan and Glasser.[8] In the same unrestricted HF approximation, MacDonald, Oji, and Bryant[13] studied the behavior of the ground state of an electron gas confined in a superlattice potential when a strong magnetic field is applied perpendicularly to the interfaces. They found that the electron-electron interaction favors the localization of the electronic charge in individual wells and the formation of a crystalline structure, perpendicular to the magnetic field, inside the wells. From the results of these works[12,31] and from our results, we infer that this state has a modulation of the charge in the z direction at the time that the electron gas forms a crystalline structure in the x-y plane. We think that the modulation of the charge in the z direction is the equivalent to the formation of CDW in the Kaplan-Glasser rods,[31] and is the equivalent to the localization of the charge in individual wells in the superlattice case.[13]

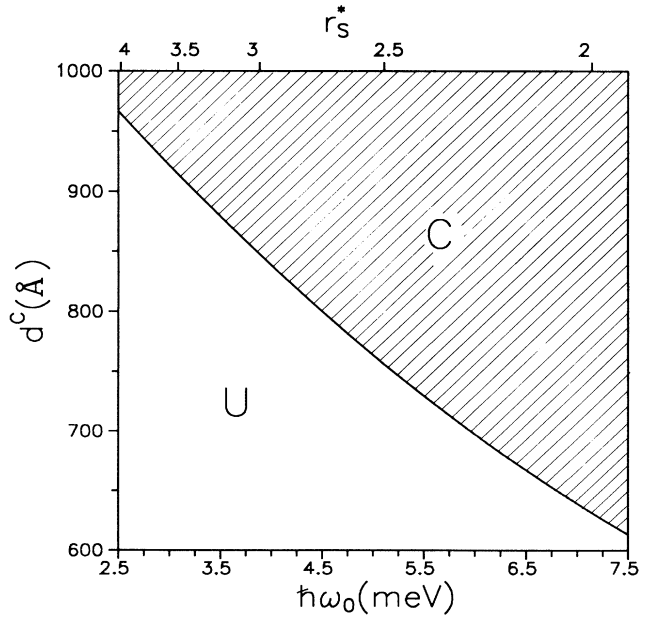

FIG. 7. Variation of the critical thickness d^C for a phase transition to a charge-density-wave state (see text) as a function of the curvature of the parabolic potential. The shaded part denotes the region where the CDW instability occurs.

In order to check the dependence of our results on the parabolic form of the well, we have studied the variation of the critical thickness d^C of a parabolic well of $\hbar\omega_0$=2.92 meV, when a potential of the form[32,33]

$$V_{\rm SL} \cos\left(2\pi \frac{z}{d_{\rm SL}}\right)$$

is added to the quadratic potential. We have fixed $d_{\rm SL}$ to 200 Å and we have varied $V_{\rm SL}$ and find that d^C is nearly independent of $V_{\rm SL}$ in the range between zero and 40 meV. Thus we expect that our results, obtained for a parabolic potential, can be generalized to other shapes of the confining potential. For instance, we think that this instability has the same nature as that found in a double-quantum-well structure.[15]

It must be emphasized that our calculations should be applied with some caution to current experiments, because the effects of impurities have been completely neglected in our model and because in the HF approximation we are neglecting correlation effects. We expect that higher corrections to the HF approximation only have the effect of screening the Coulomb interaction and then change the phase boundary line in Fig. 7 to higher d^C. We think that our calculations provides some ideas about the properties of a quasi-3DEG in presence of a perpendicular magnetic field and it could be a starting point for further analysis. In particular a natural improvement of our approach would be the so-called unrestricted Hartree-Fock approximation, in which the density of electrons is not restricted to be uniform in the x-y plane.

We are going to finish this section by commenting briefly on the possible consequences on the transport properties of the existence of a crystalline structure in the x-y plane. This state, due to the periodicity in the x-y plane, is expected to have a gap in the excitation spectrum. But this gap does not allow the existence of a plateau in the Hall resistance since one might expect this new periodicity to become pinned by the impurities. We think that this is the reason why in some magnetotransport experiments in double-

quantum-well structures[11] and in wide simple-quantum-well structures[34] the plateau $\nu=1$ is missed. However, from the published magnetotransport experiments in WPQW, we do not infer the loss of the $\nu=1$ plateau in the QHE. Only in the Fig. 5.3a of Ref. 35, we observe a not very well formed plateau at $\nu=1$ for a density of electrons $n_s/n_0 \sim 2000$ Å. However, these weak QHE features at $\nu=1$ become stronger[36] as the temperature was lowered below 100 mK. This last experiment corresponds to the wider electronic layer obtained in WPQW. We have mentioned that correlation effects could make, in Fig. 7, the phase line separation change a higher d^C; then we think that more experimental work on the variation of the $\nu=1$ plateau in the QHE with the electron gas thickness is needed.

V. SUMMARY

We have studied the dispersion relation of spin- and charge-density excitation of a parabolic-quantum-well system. We have found the following. (i) The $q=0$ lowest-energy excitation of this system corresponds to spin-density excitations. In the limit $q \rightarrow \infty$ and for low density of electrons in the system the lowest-energy gap is a SDE and changes to a CDE when the thickness of the electron layer is around 500 Å. (ii) The system undergoes a phase transition, to some kind of ordered phase as the thickness of the electron gas increases. We suggest that this phase transition could produce the destruction of the $\nu=1$ plateau in the QHE.

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