Energy Spectrum and Charge-Density-Wave Instability of a Double Quantum Well in a Magnetic Field

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Treating the electrons in the Hartree-Fock approximation, we study the wave-vector dependence of the spin-density excitations and the charge-density excitations of a double-quantum-well (DQW) system in a strong magnetic field with total $\nu=1$. We conclude that as the distance between the wells increases, the DQW system undergoes a phase transition, probably to a charge-density-wave state. We discuss the possible effects of this phase transition on the quantum Hall effect.

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The study of a high-mobility two-dimensional electron gas (2DEG) under strong magnetic fields B applied perpendicular to the electron layer has led to the discovery of the integer[1] and the fractional[2] quantum Hall effects (QHE's). Recently, the study of the evolution of the QHE states of a quasi-2DEG when the third dimension is introduced has received much attention. This degree of freedom can be introduced into the system in different ways: by means of a new periodicity (superlattice) in the third direction,[3] by growing a wide parabolic quantum well,[4] or by fabricating a double quantum well[5] (DQW).

Recently, Boebinger *et al.*[5] have reported magnetotransport measurements in DQW's. These experiments show the absence of some plateaus in the integral QHE. In particular, it is reported[5] that as the barrier thickness between the two wells increases, the integer plateau corresponding to the Hall resistance h/e^2 is destroyed. This state corresponds to the filling factor $\nu=1$ of the *total* 2D density of electrons. In Ref. 5, the $\nu=1$ state was associated with the symmetric-to-antisymmetric (SAS) gap of the DQW and it was concluded[5] that high magnetic fields applied perpendicular to the quantum wells can destroy this SAS gap.

In addition, several theoretical studies[6-9] on a model of two parallel 2DEG's coupled by the Coulomb interaction have been performed. In this model of the DQW system (which we will call the δ model) the electrons are δ-function localized in the direction perpendicular to the 2DEG and tunneling between layers is not allowed. Numerical results[6,7] on this model suggest that in the case of $\nu=1$, and for distances between layers around twice the magnetic length $l=\sqrt{\hbar c/eB}$, the Coulomb interaction between electrons in different layers produces a unique ground state and opens a gap in the energy spectrum, making possible the existence of the QHE. In the same model and in the Hartree-Fock approximation Fertig[8] has studied the charge-density excitations (CDE's) of the *normal* state, in the case of $\nu=1$. By *normal* state we mean a uniform distribution of the electron charge equally divided between the two layers, and with single-particle energies obtained self-consistently from the Hartree-Fock equations. Fertig[8] showed that as the separation between the 2DEG's increases, the dispersion relation of the CDE develops a minimum at a wave vector on the order of the inverse of the magnetic length. This minimum becomes a soft mode for layers which are separated by a distance on the order of the magnetic length. Note that in the absence of tunneling the energy spectrum corresponding to the CDE tends to zero with the wave vector.[8] Therefore, the δ model is expected to be a gapless system in the *normal* state and will undergo a phase transition when the distance between the layers increases. A generalization of the δ model, in which a SAS gap is simulated, has been reported recently by MacDonald, Platzman, and Boebinger.[9] These authors[9] studied the CDE of this model in the single-mode approximation and found that the system undergoes a phase transition as the barrier between the electron layers increases. They argue that this transition destroys the SAS gap, and therefore the QHE.

In this paper we study the electronic properties of a more realistic DQW system in the presence of a strong perpendicular magnetic field corresponding to $\nu=1$. We treat the electrons in the effective-mass approximation. The barrier between the wells has a height V_b and a thickness d_b. Tunneling between wells is inherently included in this model. We calculate the eigenstates and eigenvalues of the *normal* state of the system in the Hartree-Fock approximation, and investigate the CDE and the spin-density excitations (SDE's) of the system using the self-consistent approximation discussed by Kallin and Halperin[10] and applied by Fertig[8] to the δ model. In this approximation, the existence of soft modes indicates that the system undergoes a phase transition.

In the Hartree-Fock approximation, with the magnetic field applied in the z direction, with $\nu=1$, and assuming translational invariance in the (x,y) plane, the wave

functions and the self-energies of the *normal* state take the form[11]

$$\Psi_{i,k_y,\sigma}(\mathbf{r}) = \frac{1}{\sqrt{L_y}} e^{ik_y y} \varphi_0(x - k_y l^2) \chi_{i,\sigma}(z) U(\sigma) , \quad (1a)$$

$$\varepsilon_{i,k_y,\sigma} = \tfrac{1}{2}\hbar\omega_c + E_{i,\sigma} . \quad (1b)$$

Here L_y is the dimension of the sample in the y direction, φ_0 is the lowest eigenstate of the one-dimensional harmonic oscillator, σ is the electron-spin variable[12] $(\uparrow,\downarrow)$, $U(\sigma)$ is the spin-wave function, $\omega_c = eB/m^*c$ is the cyclotron frequency, m^* is the electron effective mass, and $E_{i,\sigma}$ and $\chi_{i,\sigma}$ are obtained from

$$[-g^*\mu_B B S_z + V(z) + V_H(z)]\chi_{i,\sigma}(z) - \frac{e^2}{\epsilon}\frac{1}{l}\left(\frac{\pi}{2}\right)^{1/2} \int dz' e^{|z-z'|^2/2l^2} \operatorname{erfc}\left(\frac{z-z'}{\sqrt{2}l}\right) \chi_{s,\sigma}(z')\chi_{i,\sigma}(z')\chi_{s,\sigma}(z) = E_{i,\sigma}\chi_{i,\sigma}(z) . \quad (2)$$

In this expression g^* is the effective Landé factor, μ_B is the Bohr magneton, S_z is $\frac{1}{2}$ for[12] $\sigma = \uparrow$ and $-\frac{1}{2}$ for $\sigma = \downarrow$, ϵ is the dielectric constant, erfc is the complementary error function, $V(z)$ is the manmade potential, $V_H(z)$ is the Hartree potential, and the last term in Eq. (2) corresponds to the exchange self-energy. The index s stands for the symmetric state.

Solving Eq. (2) and the Hartree potential V_H self-consistently, we obtain $E_{i,\sigma}$ and $\chi_{i,\sigma}(z)$; this allows us to calculate the CDE and the SDE's of the system. The SDE's correspond to excitons where the electron and the hole have different spin orientations, and therefore the energies of the SDE come from the poles of the spin-density response function. In the self-consistent approximation,[10] working in the lowest Landau level and taking into account only the symmetric and antisymmetric states, we find that the frequencies of the SDE are given by

$$\hbar\omega_i^S(q) = E_{i,\downarrow} - E_{s,\uparrow} - \tilde{V}_{s\uparrow,i\downarrow,s\uparrow,i\downarrow}(q) , \quad (3)$$

where q is the wave vector of the excitation, i can be s (symmetric), or a (antisymmetric), and

$$\tilde{V}_{i\sigma',j\sigma,k\sigma',l\sigma}(q) = \frac{e^2}{\epsilon}\int_0^\infty dk\, e^{-k^2l^2/2} J_0(kql^2) \int dz\, dz'\, e^{-k|z-z'|} \chi_{i,\sigma'}(z)\chi_{j,\sigma}(z')\chi_{k,\sigma'}(z)\chi_{l,\sigma}(z') , \quad (4)$$

where J_0 is a Bessel function. The excitation of frequency $\omega_s^S(q)$ corresponds basically to an exciton in which the electron and the hole reside in the symmetric state but with different spin orientation. Similarly, the branch $\omega_a^S(q)$ describes an exciton in which the hole is in the symmetric state with spin parallel to the field and the electron resides in the antisymmetric state with spin antiparallel to the magnetic field.

The CDE corresponds to excitons where the electron and the hole have the same spin orientation; therefore the energies of the CDE come from the poles of the charge-density response function. Using the same approximations as for the SDE case, we obtain that the frequency corresponding to the CDE is

$$\hbar\omega^C(q) = \{[E_{a,\uparrow} - E_{s,\uparrow} - \tilde{V}_{s\uparrow,a\uparrow,s\uparrow,a\uparrow}(q) + \tilde{V}_{a\uparrow,a\uparrow,s\uparrow,s\uparrow}(q)] \times [E_{a,\uparrow} - E_{s,\uparrow} - \tilde{V}_{s\uparrow,a\uparrow,s\uparrow,a\uparrow}(q) - \tilde{V}_{a\uparrow,a\uparrow,s\uparrow,s\uparrow}(q) + 2V_{a\uparrow,s\uparrow,s\uparrow,a\uparrow}(q)]\}^{1/2} , \quad (5)$$

where

$$V_{i\sigma,j\sigma,k\sigma,l\sigma}(q) = \begin{cases} \dfrac{e^2}{\epsilon}\dfrac{1}{ql^2} e^{-q^2l^2/2} \displaystyle\int dz\, dz'\, e^{-q|z-z'|} \chi_{i,\sigma}(z)\chi_{j,\sigma}(z')\chi_{k,\sigma}(z)\chi_{l,\sigma}(z') & \text{if } q \neq 0, \\ -\dfrac{e^2}{\epsilon}\dfrac{1}{l^2} \displaystyle\int dz\, dz'\, |z-z'| \chi_{i,\sigma}(z)\chi_{j,\sigma}(z')\chi_{k,\sigma}(z)\chi_{l,\sigma}(z') & \text{if } q = 0. \end{cases} \quad (6)$$

The excitation frequency $\omega^C(q)$ describes an exciton in which the hole and the electron have the same spin orientation, but they reside in the symmetric and antisymmetric state, respectively.

We study the SDE and the CDE as a function of the wave vector of the excitation and the thickness of the barrier d_b. The parameters we have used for the calculation are $m^* = 0.067$, $\epsilon = 12.5$, $g^* = 0.44$, and $V_b = 250$ meV. The two-dimensional density of electrons is $n_s = 3.8\times10^{11}$ cm^{-2} and the thickness of each well is $d_w = 139$ Å. The background of positive charge consists of two uniform layers of equal charge density, 200 Å thick, and is located 250 Å from either outer edge of the DQW structure.

In Fig. 1 we show, as a function of d_b, the energies corresponding to the $q = 0$ SDE's $[\omega_{s,a}^S(q=0)]$ and CDE $[\omega^C(q=0)]$. This figure shows that as required by Larmor's theorem the energy $\hbar\omega_s^S(q=0)$ is independent of d_b and equal to the Zeeman energy $|g^*\mu_B B|$. For the same reason $\hbar\omega_a^S(q=0) = |g^*\mu_B B| + \Delta_{\mathrm{SAS}}^0$, where Δ_{SAS}^0 is the one-electron SAS gap which decreases exponen-

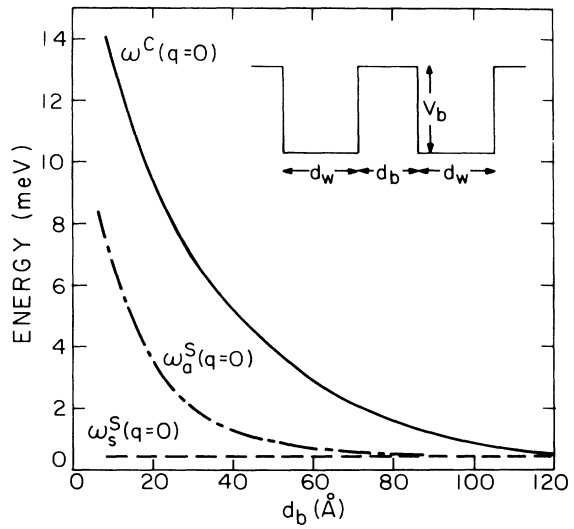

FIG. 1. Variation of the $q=0$ excitations of a DQW system as a function of the thickness of the barrier d_b. The parameters of the calculation are given in the text. Inset: DQW system shown schematically.

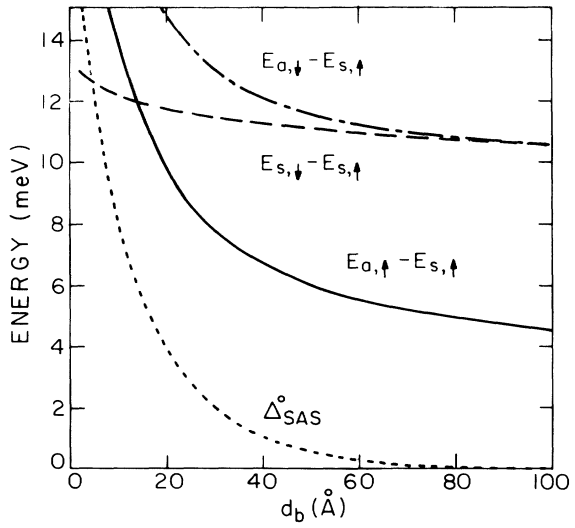

FIG. 2. Variation of the $q\rightarrow\infty$ excitations of a DQW system as a function of the thickness of the barrier d_b. The parameters of the calculation are given in the text. Also plotted is the variation of Δ^0_{SAS} gap as a function of d_b.

tially with d_b. As expected we find that the frequency corresponding to the $q=0$ CDE depends strongly on the separation between the wells. The limit corresponding to the δ model [$\omega^C(q=0)\rightarrow 0$] is obtained when $d_b \gg d_w$. Only in this limit there is an exact cancellation[8] between the Hartree-Fock enhancement of the SAS gap and the vertex corrections $\tilde{V}$, and then $\omega^C(q=0)\rightarrow 0$. In other cases, $\omega^C(q=0)$ is strongly dependent on the electron-electron interaction, and is generally larger than Δ^0_{SAS}. This is why, for thicknesses of the barrier smaller than 120 Å, the energies corresponding to SDE are lower in energy than those corresponding to CDE (see Fig. 1).

In Fig. 2 we show the $q\rightarrow\infty$ limit of the SDE's and CDE. In this limit, the exciton consists of an electron and a hole infinitely separated,[10] thus the corrections V and $\tilde{V}$ are zero, $\omega^C(q)=E_{a,\uparrow}-E_{s,\uparrow}$, $\omega_s^S(q)=E_{s,\downarrow}-E_{s,\uparrow}$, and $\omega_a^S(q)=E_{a,\downarrow}-E_{s,\uparrow}$. The lowest of these gaps is responsible for the plateau $\nu=1$ in the QHE. These three gaps decrease with d_b, but the gap corresponding to the CDE decays faster than those corresponding to the SDE's. Thus we obtain that, for large values of ql and small values of d_b, the lowest gap is a SDE but for larger values of d_b the smallest gap is the CDE corresponding to the SAS transition. This transition occurs at a distance between the wells of around 18 Å. Note that, due to the self-energy corrections [Eq. (2)], the gap $E_{a,\uparrow}-E_{s,\uparrow}$ is considerably bigger than the one-electron SAS gap Δ^0_{SAS} (see Fig. 2). Since at large d_b, this gap is responsible for the plateau $\nu=1$ in the QHE, we conclude that in the *normal* state, even for very small Δ^0_{SAS}, it is possible to observe this plateau in the transverse magnetoresistance.

In Fig. 3 the wave-vector dependence of the CDE and SDE's of the system is shown for two values of d_b. For $ql\ll 1$, the energy spectrum corresponding to the SDE's [$\omega^S_{s,a}(q)$] varies quadratically with ql. This behavior is the same for different thicknesses of the barrier and is of the form one expects for spin-flip excitations.[10] The difference in energies between the symmetric and antisymmetric SDE's is around Δ^0_{SAS}, and is practically independent of the wave vector q. More interesting is the behavior of the energy spectrum of the CDE [$\omega^C(q)$]. For $ql<1$ the dispersion relation decreases with the wave vector, developing a minimum at values $ql\sim 1.5$. By increasing the distance between the wells this minimum becomes deeper [Fig. 3(b)] and for separations between the wells larger than a critical distance d_b^c the dip becomes a soft mode which indicates that the system undergoes a phase transition. For the parameters we are using, we have found $d_b^c\sim 23$ Å.

The fact that for a certain d_b^c and for a certain wave vector q^c the frequency ω^C becomes zero implies that the static charge-density response function of the DQW system diverges at this wave vector, and therefore that the system is unstable against the formation of charge-density waves (CDW's) of wave vector q. Then, we expect that the phase transition we have found leads the system to some kind of Wigner crystal. We believe this is also the case in the works of Fertig[8] and MacDonald, Platzman, and Boebinger.[9] This new CDW state 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 the CDW to become pinned by the impurities. Thus, we conclude that the vanishing of the plateau $\nu=1$ in the experiment of Ref. 5 can be understood by means of this phase transition.

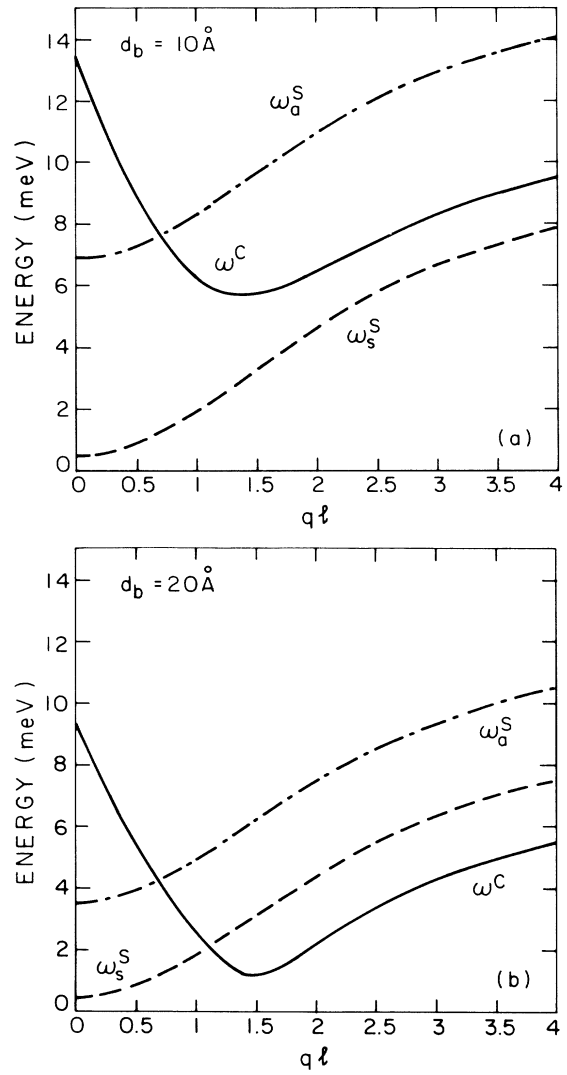

FIG. 3. Dispersion relation of the CDW (ω^C) and the SDE's ($\omega_{s,a}^S$) for a DQW system with (a) $d_b = 10$ Å and (b) $d_b = 20$ Å. The parameters of the calculations are given in the text.

The calculated critical distance d_b^c, where the phase transition occurs, is smaller than the experimental value where the $\nu = 1$ plateau disappears. But we think that the agreement between the experiment and our calculation is good enough and shows that our theory retains the more important features of the physics of the problem.

In conclusion, we have found the following for a set of parameters describing the DQW of Ref. 5: (i) The $q = 0$ lowest energy excitation of the DQW system corresponds to spin-density excitation. In the limit of $q \to \infty$ and for small d_b the lowest energy gap is a SDE, and changes to a CDE when the distance between the wells is around 18 Å. (ii) The system undergoes a phase transition, probably to a Wigner crystal, as the separation between the wells increases. This phase transition occurs at $d_b^c \sim 23$ Å. We suggest that this phase transition is responsible for the destruction of the plateau $\nu = 1$ in the QHE experiments.[5]

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[11]We use the fact that in the *normal* state the (x,y)-dependent part of the single wave function is the same in the case of independent electrons as in the Hartree-Fock approximation.

[12]We have assumed that the electron g^* factor is positive. In the cases where g^* is negative, as in GaAs, the role of $\uparrow$ and $\downarrow$ must be interchanged in our equations.