Broken-symmetry ground states for the two-dimensional electron gas in a double-quantum-well system

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Working in the Hartree-Fock approximation, we calculate the ground-state energy of different states of the two-dimensional electron gas in a double-quantum-well system as a function of the separation of the wells. Our calculation takes tunneling between the wells as well as the finite thicknesses of the wells into account. In the absence of interlayer hopping the ground state at small layer separations has a spontaneously broken symmetry in which hopping matrix elements have nonzero expectation values. We find that, as the separation of the wells is increased to some critical distance d_c, the Hartree-Fock ground state breaks translational symmetry and the hopping order parameters rapidly diminish.

I. INTRODUCTION

A two-dimensional electron gas (2DEG) exhibits a variety of phenomena when subjected to a strong perpendicular magnetic field. The integral[1] and fractional[2] quantum Hall effects are observed at integer values of the filling factor ν and at some specific fractional values of ν. Below some critical filling factor of order $\nu \approx 0.2$, the electron gas is expected to condense into a Wigner crystal.

Recent advances in material-growth technology allow the fabrication of multiple two-dimensional electron layers in close proximity. This introduces new degrees of freedom associated with the third dimension. The simplest of these structures is the double-quantum-well system (DQWS) in which two interacting electron-electron or electron-hole layers are separated by a distance d. It is particularly interesting to study the evolution of the ground state of such a system, as the well separation is varied, since a variety of new phases are then possible. In particular, it has been predicted that the electron-electron interaction among the two layers of the DQWS will lead to fractional quantum Hall states with even denominators[3,4] and to increased stability of the Wigner crystal state.[5-10]

For a pair of identical quantum wells with interwell tunneling, the symmetric-to-antisymmetric gap Δ_{SAS} can be controlled experimentally and is usually much smaller than the Landau-level spacing. In the strong-field limit, Δ_{SAS} is typically of the order of the Coulomb interaction. When Coulomb effects are neglected in this limit, the excitation gap at odd-integer filling factors is Δ_{SAS} and results in a quantum Hall state. It was shown theoretically[7] that when Coulomb interaction is added to the picture, the Coulombic gain in intralayer interactions as the well separation is increased can exceed costs in hopping energy and interlayer interaction energy, leading to a collapse of the excitation gap, which results in the disappearance of the quantum Hall effect. This was observed experimentally[11] at filling factors $\nu = 1, 3$. The collapse of the SAS gap is also reflected in a vanishing energy for a collective excitation of the uniform state of the DQWS at some critical separation d_c at momentum vector q_c.[6,8] This softening suggests that the 2DEG in the DQWS becomes unstable against the formation of some kind of charge-density-wave (CDW) state, or even a Wigner-crystal (WC) state. (As we discuss below, these states of broken translational symmetry may be preempted by strongly correlated fluid states in which translational invariance is restored by quantum fluctuations.)

In fact, because Coulomb interactions can lead to mixing of the electronic states of the two wells, a more complex kind of CDW or WC state is possible. For a DQWS consisting of spatially separated electron and hole layers, it was shown[9] that, above some critical separation, the new ground state contains, besides the density modulation of the CDW state, a Bose condensate of electron-hole pairs at $q = 0$ as well as at the wave vectors of the CDW state. This novel kind of correlated state was called an excitonic charge-density-wave state. In the strong-magnetic-field limit, electron-electron systems can be related to electron-hole systems by making a particle-hole transformation in one of the two layers.[6,12] The excitonic order of electron-hole systems corresponds in electron-electron systems to order in which electrons tend to exist in a particular linear combination of the two

isolated-well single-particle states even when there is no hopping between the wells. We will refer to states with this type of order as coherent states. If we make a spin-$\frac{1}{2}$ analogy for the well degree of freedom as in Ref. 7, where states localized in left and right layers are associated with eigenstates of a Pauli spin operators (for definiteness say σ_x) with eigenvalues ± 1, respectively, the Hamiltonian of the system can be shown to be invariant under rotations about the x axis in spin space. As we discuss in more detail below, electrostatics favor a ground state with $S_x^{\rm tot}=0$ (equal numbers of electrons in the two layers), while exchange tends to favor spin polarization in the y-z plane. In this language, the broken symmetry is seen to be a $U(1)$ symmetry, corresponding to the choice of orientation in the y-z plane for the total spin.

In this paper, we investigate the nature of the ground state of the electron-electron DQWS above the critical separation where CDW and Wigner-crystal states are expected to occur. We calculate, in the Hartree-Fock approximation, the energy of different possible nonuniform states, specifically including CDW, WC, and coherent states. Our method for calculating the energy of the crystal states is based on a numerical technique developed in Ref. 13, which is valid in the strong-magnetic-field limit. We include in our calculation the tunneling of electrons between the two wells and also the thickness of the wells. We show that, above some critical separation $d_c \approx 1.2l$, the Hartree-Fock ground state of the DQWS breaks translational symmetry in forming a coherent WC state consisting of two shifted square lattices. The coherent character of this state disappears quickly, however, as the separation is increased, and, at larger separation, the ground-state evolves into two shifted square Wigner lattices with no coherent character.

This paper is organized as follows. In Sec. II we describe the approximations used to describe the DQWS and derive the Hartree-Fock Hamiltonian of the 2DEG in the strong-field limit. In Sec. III, we derive the equation of motion of the one-particle Green's function from which we extract the ground-state densities $\langle n(\mathbf{q})\rangle$. These densities can be considered as the order parameters for the different possible states that we define in Sec. IV. We present our numerical results in Sec. V and conclude in Sec. VI.

II. HARTREE-FOCK HAMILTONIAN OF THE 2DEG IN THE DQWS

The system that we consider in this paper consists of two quantum wells of equal width b separated by a distance d measured from the center of one well to the center of the other. Two neutralizing uniform positive backgrounds are located at distance s from the center of each well. In the experiment of Ref. 11, where the disappearance of some quantum Hall plateaus are observed, $b=139$ Å, $s=600$ Å, and $d-b$ takes the values 28, 40, and 51 Å.

A magnetic field $\mathbf{B}=-B_0\hat{z}$ is applied in the direction perpendicular to the wells. In the Landau gauge, the eigenstates of the kinetic-energy operator have the form

$$\phi_{nXj}(\mathbf{r})=\frac{1}{\sqrt{L_y}}e^{iXy/l^2}\phi_n(x-X)Z_j(z)\ , \tag{1}$$

where $\phi_n(x)$ are the one-dimensional harmonic-oscillator eigenstates, $l=(\hbar c/eB_0)^{1/2}$ is the Larmor radius, and, for a finite system, the allowed values of the quantum number X are separated by $2\pi l^2/L_y$. The energy eigenvalues of the Landau levels n are given by $\epsilon_n=(n+\frac{1}{2})\hbar\omega_c$, where $\omega_c=eB_0/m^*c$ (m^* is the effective mass of the electrons) and are independent of X. The degeneracy of each Landau level is thus given by $g=S/2\pi l^2$, where S is the area of the two-dimensional electron gas in each well. We define the filling factor of the *entire* DQWS as $\nu=N/g$, where N is the total number of particles in both wells. (We assume that the two wells are equally filled.) Finally, $Z_j(z)$ ($j=1$ or 2 for the well to the left or right of $z=0$) is the wave function of the electrons in the direction perpendicular to the plane of the wells and will be defined below.

In order to get a manageable problem, we make the usual approximation[6–8] of keeping only one electronic state in each well. In the presence of tunneling, these two states mix into symmetric and antisymmetric combinations separated by an energy gap $\Delta_{\rm SAS}$. In the strong-field limit, this energy gap is much smaller than the Zeeman energy, and for filling factor $\nu\le 2$, the ground state is assumed to be fully spin polarized. (We will also consider, later on, the case $\nu=3$ in order to compare our results with those of Ref. 11. We will then comment more on the generalization of our formalism to that case.) In the strong-field limit, $\hbar\omega_c \gg \Delta_{\rm SAS}$, so that we can also make the lowest-Landau-level approximation (LLLA) of keeping only the $n=0$ Landau level. With these approximations, the density operator can be written as

$$n(\mathbf{r},z)=\sum_{X,X'}\sum_{j,j'}\phi_X^*(\mathbf{r})\phi_{X'}(\mathbf{r})Z_j^*(z)Z_{j'}(z)c_{Xj}^\dagger c_{X'j'}\ . \tag{2}$$

It is convenient to define the operator

$$\rho_{jj'}(\mathbf{q})=g^{-1}\sum_{X,X'}e^{-(i/2)q_x(X+X')}\delta_{X,X'-q_yl^2}c_{Xj}^\dagger c_{X'j'}\ , \tag{3}$$

so that the Fourier transform of the density operator can be written as

$$n(\mathbf{q},z)=g\sum_{j,j'}e^{-q^2l^2/4}Z_j^*(z)Z_{j'}(z)\rho_{jj'}(\mathbf{q})\ . \tag{4}$$

The operator $\rho_{ij}(\mathbf{q})$ obeys, in the LLLA, the commutation relation

$$g[\rho_{ij}(\mathbf{q}),\rho_{kl}(\mathbf{q}')]=\delta_{jk}\rho_{il}(\mathbf{q}+\mathbf{q}')e^{i(\mathbf{q}\times\mathbf{q}')l^2/2}-\delta_{il}\rho_{kj}(\mathbf{q}+\mathbf{q}')e^{-i(\mathbf{q}\times\mathbf{q}')l^2/2}\ , \tag{5}$$

where we use the two-dimensional cross product as a short form for $\mathbf{q}\times\mathbf{q}'\equiv q_xq_y'-q_yq_x'$.

Making the Hartree-Fock pairing of the electron operators in the Hamiltonian of the two-dimensional electron gas, we obtain the result

$$H=g\sum_j \epsilon\rho_{jj}(0)-gt[\rho_{12}(0)+\rho_{21}(0)] +g\left[\frac{e^2}{\epsilon_0 l}\right]\sum_{ijkl}\sum_{\mathbf{q}}[H_{ijkl}(\mathbf{q})-X_{ilkj}(\mathbf{q})] \times\langle\rho_{ij}(-\mathbf{q})\rangle\rho_{kl}(\mathbf{q}) , \quad (6)$$

where ϵ_0 is the dielectric function of the host semiconductor, t is the tunneling parameter (which is an implicit function of the well separation to be defined later), and ϵ is the energy of the noninteracting state defined in Eq. (1).

The usual HFA for the homogeneous electron gas is obtained by simply setting all $\langle\rho_{ij}(\mathbf{q})\rangle=0$ for $\mathbf{q}\neq 0$ in Eq. (6). The quantities $\langle\rho_{ij}(\mathbf{q})\rangle$ can in fact be interpreted as the "order parameters" of the nonhomogeneous state and will be discussed in Sec. IV.

The effective Hartree (H) and Fock (X) interactions in Eq. (6) are defined by

$$H_{ijkl}=\frac{1}{2\pi e^2 l/\epsilon_0}e^{-q^2l^2/2}\Gamma_{ijkl}(\mathbf{q}) , \quad (7)$$

and

$$X_{ijkl}(\mathbf{q})=\frac{l\epsilon_0}{e^2}\int\frac{d\mathbf{q}'}{(2\pi)^2}e^{-iq'^2l^2/2}e^{-i\mathbf{q}\times\mathbf{q}'l^2}\Gamma_{ijkl}(\mathbf{q}') , \quad (8)$$

where

$$\Gamma_{ijkl}(\mathbf{q})=\frac{2\pi e^2}{\epsilon_0|q|}\int dz\int dz' e^{-|q||z-z'|}Z_i^*(z) \times Z_j(z)Z_k^*(z')Z_l(z') . \quad (9)$$

The HFA has been studied extensively for the case of a WC in a single quantum well.[14–17] At rational filling factors, it is possible to block diagonalize the HF Hamiltonian into blocks of finite dimension d_0, where d_0 is proportional to the number of subbands at the filling factor considered.[18] The diagonalization of these blocks is then performed numerically. If, as is the case here, we are only interested in computing the order parameters $\langle\rho_{ij}(\mathbf{q})\rangle$, a simpler numerical approach described in Ref. 13 can be employed. In this paper, we generalize this simpler approach to the case of the DQWS.

In principle, one must calculate the wave function $Z_j(z)$ by taking into account the tunneling as well as the finite width of the wells.[8] Since in this paper we work in a single-well basis instead of in the basis of the entire DQWS, we assume that the effect of the finite width of the wells approximated by taking the simple form

$$Z_j(z)=\begin{cases}\dfrac{1}{\sqrt{b}} & \text{for } |z\pm d/2|\le b/2\\ 0 & \text{otherwise,}\end{cases} \quad (10)$$

which has the merit of simplifying considerably the calculation of the effective Hartree-Fock interactions. The only nonzero elements are given by

$$V_a(\mathbf{q})\equiv H_{iiii}(\mathbf{q})=\left[\frac{1}{ql}\right]e^{-q^2l^2/2}\gamma(q,b) , \quad (11)$$

$$V_b(\mathbf{q})\equiv X_{iiii}(\mathbf{q})=\int_0^\infty d(q'l)J_0(qq'l^2)e^{-q'^2l^2/2}\gamma(q',b) , \quad (12)$$

$$V_c(\mathbf{q})\equiv H_{iijj}(\mathbf{q})=\left[\frac{1}{ql}\right]e^{-q^2l^2/2}\tilde{\gamma}(q,b,d) \quad (i\neq j) , \quad (13)$$

$$V_d(\mathbf{q})\equiv X_{iijj}(\mathbf{q})=\int_0^\infty d(q'l)J_0(qq'l^2)e^{-q'^2l^2/2}\tilde{\gamma}(q',b,d) \quad (i\neq j) , \quad (14)$$

where J_0 is a Bessel function of the first kind and we have defined the form factors

$$\gamma(q,b)=\frac{2}{bq}-\frac{2}{b^2q^2}(1-e^{-qb}) , \quad (15)$$

$$\tilde{\gamma}(q,b,d)=\frac{4}{b^2q^2}\sinh^2\left[\frac{qb}{2}\right]e^{-qd} . \quad (16)$$

We may then calculate the tunneling parameter t using an effective-mass approximation (see Sec. V). The limit of strictly two-dimensional electron layers can be recovered by letting $b\to 0$: $\gamma(q,b)\to 1$ and $\tilde{\gamma}(q,b,d)\to e^{-qd}$. In Eqs. (11)–(14), V_a and V_b are the direct (Hartree) and exchange (Fock) intrawell Coulomb interactions, while V_c and V_d are the direct and exchange interwell Coulomb interactions. These interactions are plotted in Fig. 1.

Adding to the Hamiltonian of Eq. (6) the interaction of the electrons with the positive homogeneous background, we get finally

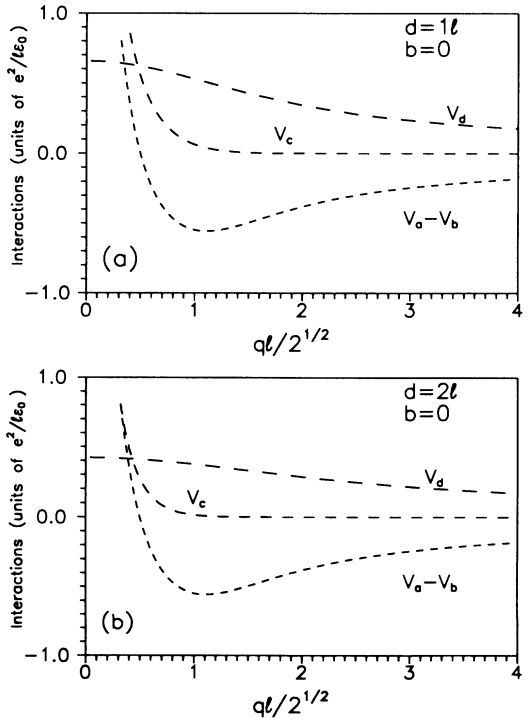

FIG. 1. Effective Hartree-Fock interactions V_a-V_b, V_c, V_d as a function of the wave vector q at well separations (a) $d=1l$ and (b) $d=2l$.

$$H=g\sum_j \epsilon' \rho_{jj}(0)-gt[\rho_{12}(0)+\rho_{21}(0)] + g\left[\frac{e^2}{\epsilon_0 l}\right]\sum_{\mathbf{q}}\sum_{ij} V_{ij}(\mathbf{q})\rho_{ij}(\mathbf{q}) , \tag{17}$$

where

$$\epsilon'=\epsilon+\left[\frac{e^2}{\epsilon_0 l}\right]\frac{\nu s}{l} , \tag{18}$$

$$V_{11}(\mathbf{q})=V_a(\mathbf{q})\langle\rho_{11}(-\mathbf{q})\rangle-V_b(\mathbf{q})\langle\rho_{11}(-\mathbf{q})\rangle + V_c(\mathbf{q})\langle\rho_{22}(-\mathbf{q})\rangle , \tag{19}$$

$$V_{12}(\mathbf{q})=-V_d(\mathbf{q})\langle\rho_{21}(-\mathbf{q})\rangle . \tag{20}$$

Note that ϵ' contains the shift of subband energies as a result of the electrostatic environment of the DQWS. This finite shift results from a cancellation between the diverging direct interactions in Eqs. (11) and (13) and the potential from the neutralizing positive backgrounds. The remaining corrections due to the finite width of the electron layers may be incorporated by setting

$$V_a(0)\equiv\frac{b}{3l} , \tag{21}$$

$$V_c(0)\equiv 0 . \tag{22}$$

V_{22} and V_{21} are obtained by interchanging the indices 1 and 2 in Eqs. (19) and (20).

III. EQUATION OF MOTION FOR $G(\mathbf{G},i\omega_n)$

We now derive the equation of motion of the single-particle Green's function

$$G_{ij}(X,X',\tau)=-\langle Tc_{iX}(\tau)c^{\dagger}_{jX'}(0)\rangle , \tag{23}$$

which is defined in such a way that its Fourier transform

$$G_{ij}(\mathbf{q},\tau)=g^{-1}\sum_{X,X'} G_{ij}(X,X',\tau)e^{-(i/2)q_x(X+X')}\delta_{X',X-q_y l^2} \tag{24}$$

is related to the order parameters $\langle\rho_{ij}(\mathbf{q})\rangle$ by the relation

$$\langle\rho_{ij}(\mathbf{q})\rangle=G_{ji}(\mathbf{q},\tau=0^-) . \tag{25}$$

Using the Hamiltonian of Eq. (17) and the Heisenberg equation of motion $\hbar\partial/\partial\tau(\cdots)=[H-\mu N,(\cdots)]$, where μ is the chemical potential and N the particle-number operator, we obtain for the equation of motion of the single-particle matrix Green's function

$$\sum_{\mathbf{q}'}\left[(i\hbar\omega_n-\epsilon'+\mu)I\delta_{\mathbf{q},\mathbf{q}'}+t\sigma_x\delta_{\mathbf{q},\mathbf{q}'} - \left[\frac{e^2}{\epsilon_0 l}\right]e^{i\mathbf{q}\times\mathbf{q}'l^2/2}V(\mathbf{q}'-\mathbf{q})\right]G(\mathbf{q}',\omega_n)=I\hbar\delta_{\mathbf{q},0} , \tag{26}$$

where I is a unit matrix in layer indices, σ_x is a Pauli matrix, and ω_n is a fermionic Matsubara frequency. Equations (25) and (26), together with the total-particle-number constraint

$$\langle\rho_{ii}(\mathbf{q}=0)\rangle=\nu/2 , \tag{27}$$

constitute a set of coupled self-consistent equations for the order parameters. These equations are very general and can, in principle, be solved at finite temperature. In this paper, however, we will only be concerned with zero-temperature solutions.

Since we are interested in CDW and WC solutions of the HF equation of motion, we allow for different stacking possibilities of the two interacting CDW or WC states. We seek solutions where the charge density in one layer is rigidly displaced with respect to the charge density in the other layer. If we take the origin of the coordinates (x,y) to be located at an inversion center in well 1, we have the relations $\langle\rho_{11}(\mathbf{r})\rangle=\langle\rho_{11}(-\mathbf{r})\rangle$ and $\langle\rho_{11}(\mathbf{r}+\mathbf{a})\rangle=\langle\rho_{22}(\mathbf{r})\rangle$, where $\mathbf{a}$ is the vector by which the CDW or WC in well 2 is shifted with respect to the CDW or WC in well 1. In Fourier space, we have

$$\langle\rho_{11}(-\mathbf{q})\rangle=\langle\rho_{11}(\mathbf{q})\rangle \tag{28}$$

and

$$\langle\rho_{22}(\mathbf{q})\rangle=e^{i\mathbf{q}\cdot\mathbf{a}}\langle\rho_{11}(\mathbf{q})\rangle . \tag{29}$$

From the definition of $\langle\rho_{12}(\mathbf{q})\rangle$, we also have the relation

$$\langle\rho_{12}(\mathbf{q})\rangle=\langle\rho_{21}(-\mathbf{q})\rangle^* . \tag{30}$$

From the equation of motion for the operators $\rho_{ij}(\mathbf{q},\tau)$, we get two more relations:

$$\langle\rho_{21}(-\mathbf{q})\rangle=e^{-i\mathbf{q}\cdot\mathbf{a}}\langle\rho_{21}(\mathbf{q})\rangle , \tag{31}$$

and, if $t\neq 0$,

$$\langle\rho_{12}(0)\rangle=\langle\rho_{21}(0)\rangle . \tag{32}$$

If $t=0$, $\langle\rho_{12}(0)\rangle$ is in general a complex number that we write as

$$\langle\rho_{12}(0)\rangle=|\langle\rho_{12}(0)\rangle|e^{i\phi} . \tag{33}$$

Using the symmetry relations derived above and redefining

$$\tilde{V}_{ij}(\mathbf{q})\equiv e^{+i\mathbf{q}\cdot\mathbf{a}/2}V_{ij}(\mathbf{q}) , \quad \tilde{G}_{ij}(\mathbf{q})\equiv e^{-i\mathbf{q}\cdot\mathbf{a}/2}G_{ij}(\mathbf{q}) , \quad \langle\tilde{\rho}_{ij}(\mathbf{q})\rangle\equiv e^{-i\mathbf{q}\cdot\mathbf{a}/2}\langle\rho_{ij}(\mathbf{q})\rangle , \tag{34}$$

Eq. (26) simplifies to a set of two coupled equations given by

$$(i\hbar\omega_n-\epsilon+\mu)\tilde{G}_{11}(\mathbf{q},\omega_n)+t\tilde{G}_{21}(\mathbf{q},\omega_n)-\left[\frac{e^2}{\epsilon_0 l}\right]\sum_{\mathbf{q}'}e^{i\mathbf{q}\times\mathbf{q}'/2}[\tilde{V}^*_{11}(\mathbf{q}-\mathbf{q}')\tilde{G}_{11}(\mathbf{q}',\omega_n)+\tilde{V}^*_{21}(\mathbf{q}-\mathbf{q}')\tilde{G}_{21}(\mathbf{q}',\omega_n)]=\hbar\delta_{\mathbf{q},0} \tag{35}$$

and

$$(i\hbar\omega_n-\epsilon+\mu)\tilde{G}_{21}(\mathbf{q},\omega_n)+t\tilde{G}_{11}(\mathbf{q},\omega_n)-\left[\frac{e^2}{\epsilon_0 l}\right]\sum_{\mathbf{q}'}e^{i\mathbf{q}\times\mathbf{q}'/2}[\tilde{V}_{21}(\mathbf{q}-\mathbf{q}')\tilde{G}_{11}(\mathbf{q}',\omega_n)+\tilde{V}_{11}(\mathbf{q}-\mathbf{q}')\tilde{G}_{21}(\mathbf{q}',\omega_n)]=0\ , \tag{36}$$

where

$$\tilde{V}_{11}(\mathbf{q})=[V_a(\mathbf{q})-V_b(\mathbf{q})+e^{-i\mathbf{q}\cdot\mathbf{a}}V_c(\mathbf{q})]\langle\tilde{\rho}_{11}(-\mathbf{q})\rangle\ , \tag{37}$$

$$\tilde{V}_{21}(\mathbf{q})=-V_d(\mathbf{q})\langle\tilde{\rho}_{12}(-\mathbf{q})\rangle\ . \tag{38}$$

In order to solve Eqs. (35) and (36) numerically, we define the "vector"

$$G(\omega_n)\equiv[\tilde{G}_{11}(\mathbf{q}_1,\omega_n),\tilde{G}_{21}(\mathbf{q}_1,\omega_n),\tilde{G}_{11}(\mathbf{q}_2,\omega_n),\tilde{G}_{21}(\mathbf{q}_2,\omega_n),\ldots,\tilde{G}_{11}(\mathbf{q}_N,\omega_n),G_{21}(\mathbf{q}_N,\omega_n)]\ , \tag{39}$$

where N is the number of order parameters taken into consideration ($\mathbf{q}_1\equiv 0$) and B is the unit vector (with $2N$ elements),

$$B\equiv(1,0,0,0,\ldots,0,0)\ . \tag{40}$$

Defining now the Hermitian matrix

$$F_{ij}=\begin{cases}-t\delta_{j,i+1}+\left[\dfrac{e^2}{\epsilon_0 l}\right]e^{i\mathbf{q}_i\times\mathbf{q}_j/2}\times\begin{cases}\tilde{V}^*_{11}(\mathbf{q}_i-\mathbf{q}_j) & \text{for } j \text{ odd and } i \text{ odd}\\ \tilde{V}^*_{21}(\mathbf{q}_i-\mathbf{q}_j) & \text{for } j \text{ even and } i \text{ odd}\end{cases}\\ -t\delta_{j,i-1}+\left[\dfrac{e^2}{\epsilon_0 l}\right]e^{i\mathbf{q}_i\times\mathbf{q}_j/2}\times\begin{cases}\tilde{V}_{21}(\mathbf{q}_i-\mathbf{q}_j) & \text{for } j \text{ odd and } i \text{ even}\\ \tilde{V}_{11}(\mathbf{q}_i-\mathbf{q}_j) & \text{for } j \text{ even and } i \text{ even}\end{cases}\end{cases} \tag{41}$$

we have, in an obvious matrix notation,

$$[(i\hbar\omega_n-\epsilon+\mu)I-F]\tilde{G}(\omega_n)=\hbar B\ . \tag{42}$$

This matrix equation can be solved by making the unitary transformation $F=UDU^\dagger$, where $UU^\dagger=I$ and D is the diagonal matrix containing the eigenvalues ω_k of F. Following Ref. 13, we have finally for the order parameters $\langle\tilde{\rho}_i\rangle$, $i=1,2,\ldots,2N$ [defined as in Eq. (39)] at $T=0$ K,

$$\langle\tilde{\rho}_i\rangle=\sum_{k=1}^{k_{\max}}U_{ik}U^*_{1k}\ , \tag{43}$$

where $k_{\max}$ can be obtained from the total-particle-number constraint

$$\langle\tilde{\rho}_1\rangle=\nu/2\ . \tag{44}$$

It is easy to show that, at $T=0$ K, we have, for the nonhomogeneous states, the sum rule

$$\sum_i|\langle\tilde{\rho}_i\rangle|^2=\langle\tilde{\rho}_1\rangle\ . \tag{45}$$

This sum rule is also valid in the homogeneous states at integer filling factors.

IV. BROKEN-SYMMETRY GROUND STATES IN THE HFA

Using the Hamiltonian of Eq. (17) and the symmetry relations derived in the preceding section, it is easy to show that the ground-state energy per electron of the two-dimensional electron gas in the DQWS is given by

$$E=E_0-\frac{e^2}{\epsilon_0 l}\left[\frac{V_b(0)\nu}{4}\right]-\frac{1}{\nu}\left[t\langle\rho_{12}(0)\rangle+t\langle\rho_{21}(0)\rangle+\frac{e^2}{\epsilon_0 l}V_d(0)|\langle\rho_{12}(0)\rangle|^2\right]$$
$$+\frac{1}{\nu}\frac{e^2}{\epsilon_0 l}\sum_{\mathbf{q}\neq 0}\{[V_a(\mathbf{q})-V_b(\mathbf{q})+\cos(\mathbf{q}\cdot\mathbf{a})V_c(\mathbf{q})]|\langle\rho_{11}(\mathbf{q})\rangle|^2-V_d(\mathbf{q})|\langle\rho_{21}(\mathbf{q})\rangle|^2\}\ , \tag{46}$$

where we have defined

$$E_0=\epsilon+\frac{e^2}{\epsilon_0 l}\left[\frac{\nu s}{2l}-\frac{\nu b}{12l}\right]\ . \tag{47}$$

Notice that this energy is (as expected from the analogy with the spin-$\frac{1}{2}$ system made in the Introduction), independent of the phase ϕ of the order parameter $\langle\rho_{12}(0)\rangle$ in the absence of tunneling. We discuss the consequences of this degeneracy in the next section.

The HF equation of motion given by Eq. (42) has a number of different solutions corresponding to different states of the electron gas in the DQWS. Each one of these solutions is characterized by a different set of order

parameters $\langle\rho_{ij}(\mathbf{q})\rangle$. As we see from Eq. (46), the ground-state energy can be expressed solely in terms of these quantities. Moreover, it is also possible to show that their knowledge is sufficient to calculate the response functions of this system.[13] To find the HF ground state we have to find the solution with minimum energy. In what follows we consider a limited number of physically interesting solutions and compare their energies. These solutions are the following:

(a) Uniform state (US): $\langle\rho_{11}(0)\rangle\neq 0$; in this solution translational symmetry is not broken and we do not allow any interwell coherence.

(b) Uniform coherent state (UCS): $\langle\rho_{11}(0)\rangle$, $\langle\rho_{12}(0)\rangle\neq 0$; in this case translational invariance is not broken but we do allow interwell coherence, which, in the absence of interwell tunneling, breaks a $U(1)$ symmetry of the Hamiltonian.

(c) Unidirectional charge-density-wave state (UCDWS): $\langle\rho_{11}(n\mathbf{G}_0)\rangle\neq 0$, $n=0,\pm 1,\pm 2,\ldots$, in this case we break translational symmetry in one direction only but do not allow interwell coherence.

(d) Unidirectional coherent CDW state (UCCDWS): $\langle\rho_{11}(n\mathbf{G}_0)\rangle$, $\langle\rho_{12}(n\mathbf{G}_0)\rangle\neq 0$, $n=0,\pm 1,\pm 2,\ldots$; now translational symmetry is broken in one direction and interwell coherence is also allowed.

(e) Wigner-crystal state (WCS) $\{\langle\rho_{11}(\mathbf{G})\rangle\}\neq 0$; in this state translational symmetry is broken in both directions. The lowest energy state of this type shares the translational symmetry of the lattice state of point electrons.

(f) Coherent Wigner-crystal state (CWCS) $\{\langle\rho_{11}(\mathbf{G})\rangle\},\{\langle\rho_{12}(\mathbf{G})\rangle\}\neq 0$; in this state interwell coherence is allowed in addition to the broken symmetry of the Wigner-crystal state.

For the Wigner-crystal solutions, $\{\mathbf{G}\}$ is a set of reciprocal-lattice vectors that defines a two-dimensional lattice with a period containing one electron.

V. NUMERICAL RESULTS

We now discuss our numerical results for the different states introduced in Sec. IV. For this discussion, we measure energies with respect to E_0, which is independent of the separation between layers and independent of the state formed by the electrons.

The US is a trivial case. The only nonzero order parameter is given by $\langle\rho_{11}(0)\rangle=\nu/2$, and the corresponding energy is independent of d. This solution corresponds to uncorrelated half-filled Landau levels in each well.

It is clear, from Eq. (46) and Fig. 1, that the UCS is lower in energy than the US even in the absence of tunneling. One can solve Eqs. (17) and (18) analytically, at filling factors $\nu=1,2$, and find that for $t\neq 0$,

$$\langle\rho_{11}(0)\rangle=\nu/2\ ,$$

$$\langle\rho_{12}(0)\rangle=\begin{cases}\mathrm{sgn}[t+V_d(0)\langle\rho_{12}(0)\rangle] & \text{if } \nu=1\\ 0 & \text{if } \nu=2\ ,\end{cases} \tag{48}$$

while for $t=0$,

$$\langle\rho_{11}(0)\rangle=\nu/2\ ,$$

$$\langle\rho_{12}(0)\rangle=\begin{cases}e^{i\phi}/2 & \text{if } \nu=1\\ 0 & \text{if } \nu=2\ .\end{cases} \tag{49}$$

These solutions are independent of the value of d. Equation (49) is a consequence of the degeneracy of the Hamiltonian with respect to the phase ϕ of the order parameter. In the following numerical results, we set this phase to be zero and also assume that $\langle\rho_{12}(0)\rangle\ll t$.

At $\nu=1$, the Landau level of symmetric states is full. This state is energetically favored over the US because when all electrons are in the symmetric combination, the Pauli exclusion principle creates an exchange hole in both interlayer and intralayer correlation functions. When t equals zero, the energy of the UCS is independent of the phase relationship between electrons in the two wells as long as it is fixed; for example, the state where all electrons are found in the antisymmetric combination of the isolated well states has precisely the same energy. This degeneracy is associated with the broken $U(1)$ symmetry discussed earlier. For d equal to zero, this Hartree-Fock ground state at $\nu=1$ is expected to be identical to the exact ground state;[19] numerical exact diagonalization studies suggest that at $\nu=1$ the UCS is a good approximation to the exact ground state for $d/l<\sim 1$. In what follows we discuss the Hartree-Fock ground state at larger values of d/l. We remark that at $\nu=1,2$ a single-particle (tunneling) gap between symmetric and an antisymmetric states exists and is given by

$$\Delta_{\mathrm{SAS}}=2\left[t+\left[\frac{e^2}{\epsilon_0 l}\right]V_d(0)|\langle\rho_{12}(0)\rangle|\right]\ , \tag{50}$$

which is a decreasing function of the well separation.

We have performed a large-scale numerical analysis of Eqs. (42)–(44) in order to find the order parameters $\langle\rho_{11}(\mathbf{q})\rangle,\langle\rho_{12}(\mathbf{q})\rangle$ in the different inhomogeneous states. For the WCS and CWCS, we find that accurately convergent results are obtained by keeping approximately 14 shells of reciprocal-lattice vectors. For the UCDWS or UCCDWS, excellent convergence is obtained with $n_{\max}=10$.

In Fig. 2(a), the energies of the UCS, UCDWS, and UCCDWS are compared for different values of d at filling factor $\nu=1$. The corresponding behavior of the order parameters is shown in Fig. 2(b), together with the Hartree and Fock contributions to the total energy. (Note that the Hartree energy vanishes in the uniform state, since it is canceled by the energy of the positive backgrounds.) We have assumed, for simplicity, $b=t=0$ and have chosen $G_0=1.2/l$ for reasons discussed below. Note that in the absence of interlayer coherence, the energy is always lowered in the Hartree-Fock approximation by breaking translational invariance. [The energy per electron of the US is $\sim -0.314(e^2/\epsilon_0 l)$, independent of the layer separation.] However, more energy is gained by breaking the $U(1)$ symmetry, and, as we have discussed above, the Hartree-Fock ground state at small layer separations is the UCS. The collective excitations of the UCS have been evaluated by Fertig[6] in the time-dependent

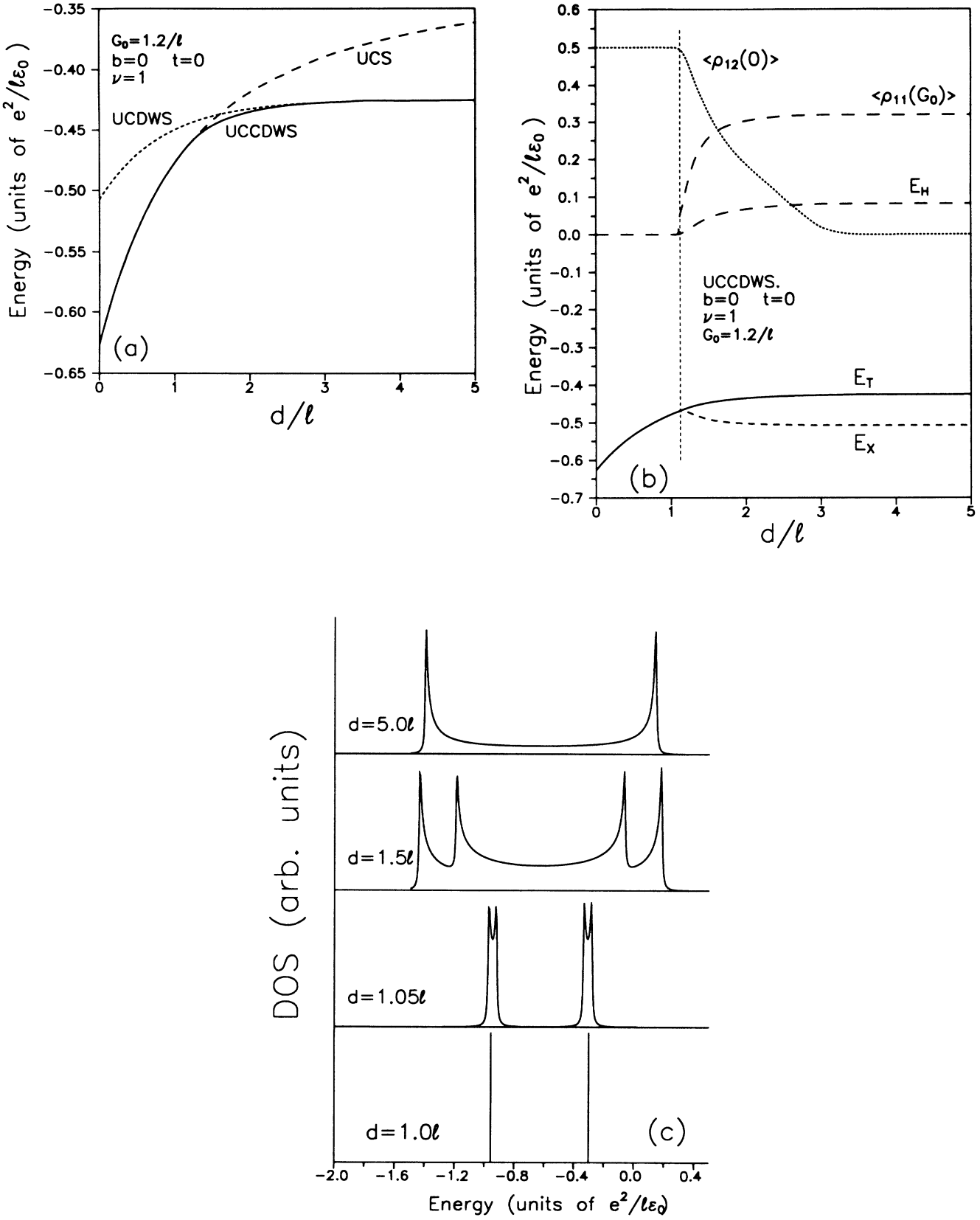

FIG. 2. (a) Ground-state energy of the UCS, UCDWS, and UCCDWS as a function of the well separation for $b=t=0$ and at filling factor $\nu=1$. (b) Order parameters $\langle\rho_{12}(0)\rangle$, $\langle\rho_{11}(0)\rangle$, and (c) density of states (DOS) of the UCCDWS of (a) as a function of the well separation. Shown in (b) are the total (E_T) and exchange (E_X) energies.

Hartree-Fock approximation and by MacDonald, Platzman, and Boebinger[7] in an approximation that reduces to the time-dependent-Hartree-Fock approximation at $\nu=1$. (For a more-thorough discussion of the consequences of symmetry breaking at $t=0$ for the collective excitation spectrum, see Wen and Zee.[20]) For $d/l > \sim 1.2$, the collective mode energies vanish for $q \sim G_0$; this instability implies that the UCS becomes unstable in the Hartree-Fock approximation for $d/l > \sim 1.2$. We see this explicitly comparing Figs. 2(a) and 2(b); as d/l crosses 1.2, the nonzero momentum order parameters become finite and the UCCDWS energy falls below that of the UCS. The driving energy for this phase transition comes from the difference between intrawell interactions and interwell interactions, which increases with the layer separations. In the UCS, intrawell and interwell correlations must be identical. At larger layer separations it becomes more important to improve intrawell correlations, and this can be accomplished only by allowing the phase relationship between electrons in different wells to fluctuate. Thus we see in Fig. 2(b) that the interlayer order parameter gets smaller as the intralayer nonzero-momentum order parameter increases. The UCDWS that we are considering here is a state in which the CDW's in the two wells are shifted by $a=\lambda/2=\pi/G_0$ with respect to one another. As for the WCS below, this is the configuration of lowest energy. The critical distance at which the UCS becomes unstable against the formation of the UCCDWS is indicated in Fig. 2(b) by the vertical dashed lines. Similar results were obtained by Chen and Quinn[9] for the electron-hole DQWS.

The density of states in the inhomogeneous states can be calculated using the relation

$$g(\omega)=\nu^{-1}\sum_k |U_{1k}|^2\delta(\omega-\omega_k)\ . \tag{51}$$

For the UCCDWS, the result is shown in Fig. 2(c) and consists of two typical one-dimensional DOS's centered at the energies of the symmetric and antisymmetric states. The separation in energy between these two states is proportional to the order parameter $\langle\rho_{12}(0)\rangle$, and their width is proportional to $\langle\rho_{11}(\mathbf{G}_0)\rangle$. Notice that for small separation between the wells, there is a gap in the single-particle density of states for the coherent phases, even in the absence of tunneling (i.e., $t=0$), due to the fact that the order parameter $\langle\rho_{12}(0)\rangle$ is not zero. The gap is a consequence of the coherent character of these states. (Note that there will be linearly dispersing gapless collective modes in these states.[6,7,20]) As the well separation increases, this order parameter decreases while $\langle\rho_{11}(\mathbf{G}_0)\rangle$ increases, so that the SAS gap disappears and the bandwidth of the one-dimensional DOS increases. In the coherent states, the existence of the SAS gap is associated with the incompressibility of the system, which is at the root of the quantum Hall effect. In the case of the UCDWS, there is no gap in the excitation spectrum, so it is not possible to observe the quantum Hall effect. The collapse of the SAS gap thus leads to the disappearance of the quantum Hall effect. For systems modulated in two directions, such as the WCS, there will be gaps in the excitation spectrum, but the densities at which they occur will not be magnetic-field dependent and the quantized Hall conductance will vanish.[21] From another point of view, we can argue that the Wigner-crystal state is expected to be pinned by impurities, so that the Hall conductivity will vanish. These systems will not exhibit the quantum Hall effect.

We now consider the Wigner-crystal states. We restrict ourselves to the hexagonal and square Wigner crystals with one electron per unit cell. In the classical case of two separated point lattices, the ground-state energy per particle [corresponding to $E-E_0$ of Eq. (46)] is given by

$$E_{\text{classical}}=\frac{e^2}{\epsilon_0 l}\left[-\alpha\left(\frac{\nu}{2}\right)^{1/2}+\sum_{\mathbf{G}\neq 0}\left(\frac{\nu}{16\pi\xi}\right)^{1/2}\frac{e^{-2\pi|\mathbf{G}|d}}{|\mathbf{G}|}\times\cos(2\pi\mathbf{G}\cdot\mathbf{a})\right], \tag{52}$$

where for a square (triangular) lattice, $\xi=1(\sqrt{3}/2)$ and $\alpha=0.777\,990(0.782\,133)$.[22] Equation (52) is a convergent expression at large enough values of d. Figure 3 shows this classical energy for the case where the two lattices are directly on top of one another ("unshifted") and where they are "shifted." (Notice that the two shifted configurations for the triangular lattice have the same energy.) As expected, the shifted lattices have lower energy than the unshifted one. At small values of d, the shifted square lattice has lower energy than the shifted triangular lattice. This situation is reversed at large values of d. Notice that the classical energy of Eq. (52) includes only the static Coulomb energy, while the Hartree-Fock energy includes, to some extent, the zero-point-motion energy of uncorrelated electrons.

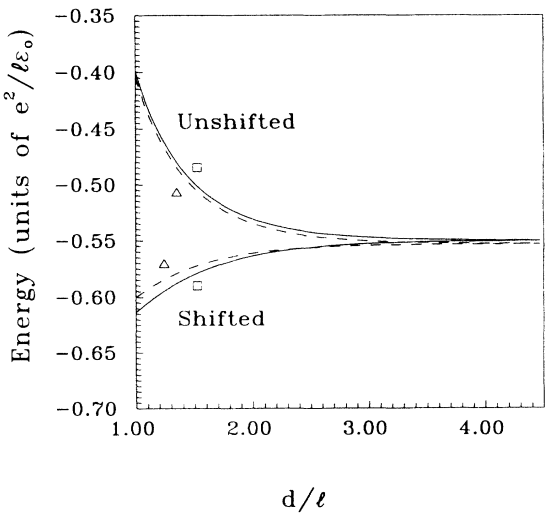

FIG. 3. Static Coulomb energy of two interacting Wigner crystals as a function of their separation. The energy is calculated in the classical approximation for the shifted and unshifted configurations (see text) of the square and triangular lattices.

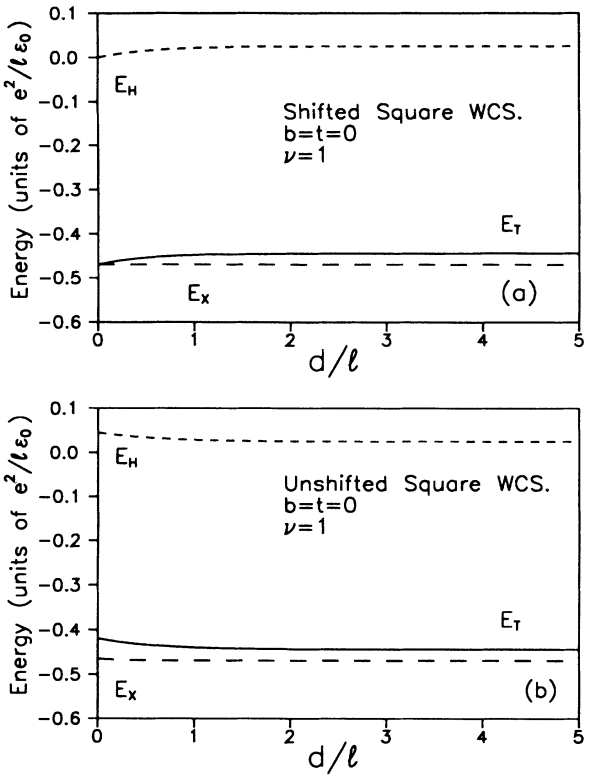

FIG. 4. Ground-state energy E_T of the (a) shifted and (b) unshifted Wigner crystal state (WCS) as a function of the well separation for $b=t=0$, $\nu=1$. Also shown are the Hartree (E_H) and exchange (E_X) contributions to the total energy.

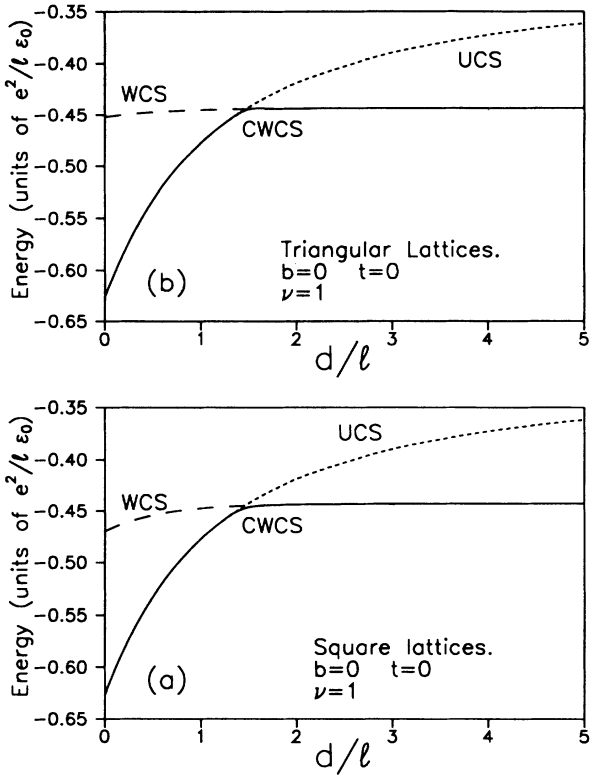

FIG. 5. Ground-state energy of the UCS, WCS, and CWCS for (a) shifted square lattices and (b) shifted triangular lattices at $b=t=0$, $\nu=1$.

Figure 4 shows the energy of the square WC for the shifted and unshifted lattices [the order parameter $\langle\rho_{12}(\mathbf{G})\rangle$ is set to zero]. As expected from the classical calculation, the shifted lattices have lower energy than the unshifted ones. This is also true for the hexagonal lattice, and we can thus consider only the shifted case from now on. The order parameter $\langle\rho_{11}(\mathbf{G})\rangle$ changes appreciably only at small values of d so that the main change in the energy comes from the interwell Hartree interaction. This can be traced back to the fact that, at filling factor $\nu=1$, the minimal value of the reciprocal-lattice vector of the Wigner crystal for the square lattice corresponds to $Gl/\sqrt{2}=1.17$. From Fig. 1, we see that, at this wave-vector value, the interwell interaction changes very little with d.

Figure 5 shows the ground-state energy for the (a) square and (b) triangular lattices at $\nu=1$ and $b=t=0$. We now allow, however, for the order parameters $\langle\rho_{12}(\mathbf{q})\rangle$ to be nonzero. When this is done, the ground state is again the UCS at small d but becomes nonuniform at large d. We see that the interlayer coherence order parameters drop to zero more abruptly once translational invariance is broken than in the case of the UCDW and UCCDW states discussed above. In the HFA (Ref. 17) and for a single well, the triangular Wigner lattice has smaller energy than the square lattice except at filling $\nu=\frac{1}{2}$, where the square lattice is slightly lower in energy. At large d (i.e., in the limit of uncoupled wells), we also observe this situation in the DQWS, although the square and triangular lattices are almost degenerate. In any case, the energy of the crystal state is lower than that of the UCDWS at large d. When the distance between the wells decreases, the difference in energy between the square and hexagonal WC's becomes bigger, and below some value of d, there is a small region where the UCCDWS has lower energy than the CWCS. So, in the absence of tunneling, the ground state of the DQWS in the Hartree-Fock approximation goes from the UCS at small d to a UCCDWS at $d/l\approx1.5$ to a square[23] CWC with very weak interlayer coherence at larger value of d.

We now introduce the tunneling in our calculation. The tunneling parameter t depends, of course, on the distance between the wells. We have calculated t in the effective-mass approximation, assuming the width of the wells to be given by its experimental value, i.e., $b=139$ Å, with a well height of 250 meV. The effective mass used in 0.067 m_0, where m_0 is the bare electronic mass. With these parameters, we have found that t can be approximated by the analytic expression

$$t=131.9e^{-0.0678d}, \tag{53}$$

where d is in Å and t is in MeV. In order to express t in units of $e^2/\epsilon_0 l$ in the equation of motion, we take the dielectric constant $\epsilon_0=12.5$ and calculate l using the relation $\nu=2\pi nl^2$, where n is the total areal density of electrons in the DQWS. For the three samples studied in Ref. 11, the interwell separations were given by $d_1=139$

Å +40 Å, $d_2=139$ Å + 51 Å, $d_3=139$ Å +28 Å, and the densities by $n_1=3.8\times10^{11}$ cm^{-2}, $n_2=3.9\times10^{11}$ cm^{-2}, $n_3=4.2\times10^{11}$ cm^{-2}. In units of the magnetic length, we thus have $d_1=2.766l$, $d_2=2.974l$, $d_3=2.712l$ at filling factor $\nu=1$, while at $\nu=3$, we have $d_1=1.597l$, $d_2=1.717l$, $d_3=1.566l$.

Figure 6(a) shows the evolution of the ground-state energy with d including interlayer tunneling for the different states at $\nu=1$. In this figure the well thickness is neglected. It is taken into account, however, in Fig. 6(b). It is quite clear that there is a region of values of d where the square CWCS is the ground state and that the main effect of adding the tunneling is to shift to higher values of d the critical well separation d_c at which the energy of the CWCS becomes lower than that of the UCS. Another effect of t is that the interlayer coherence drops more slowly with separation after translational symmetry is broken. This is due to the fact that t favors the existence of the order parameter $\langle\rho_{12}(\mathbf{q})\rangle$. From Fig. 6(b), we see that the effect of the thickness of the well is to weaken the interaction and hence to decrease the ground-state energy. Apart from a small shift d_c to higher values, the situation in that case is very similar to that of $b=0$.

In the strong-field limit where the Zeeman energy is much bigger than the SAS gap (but much smaller than the cyclotron energy), the formalism developed in this paper can easily be generalized to include the symmetric and antisymmetric states with spin opposite to the direc-

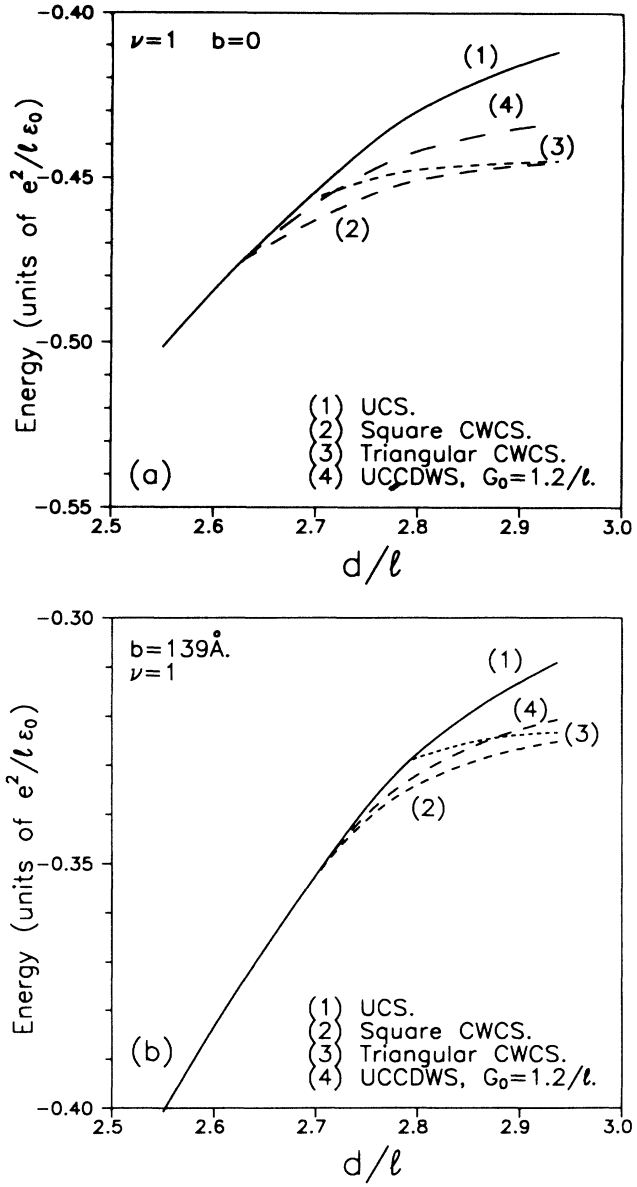

FIG. 6. Comparison of the ground-state energy as a function of the well separation of the UCS, square CWCS, triangular CWCS and UCCDWS at filling factor $\nu=1$ for (a) $b=0$ and (b) $b=139$ Å.

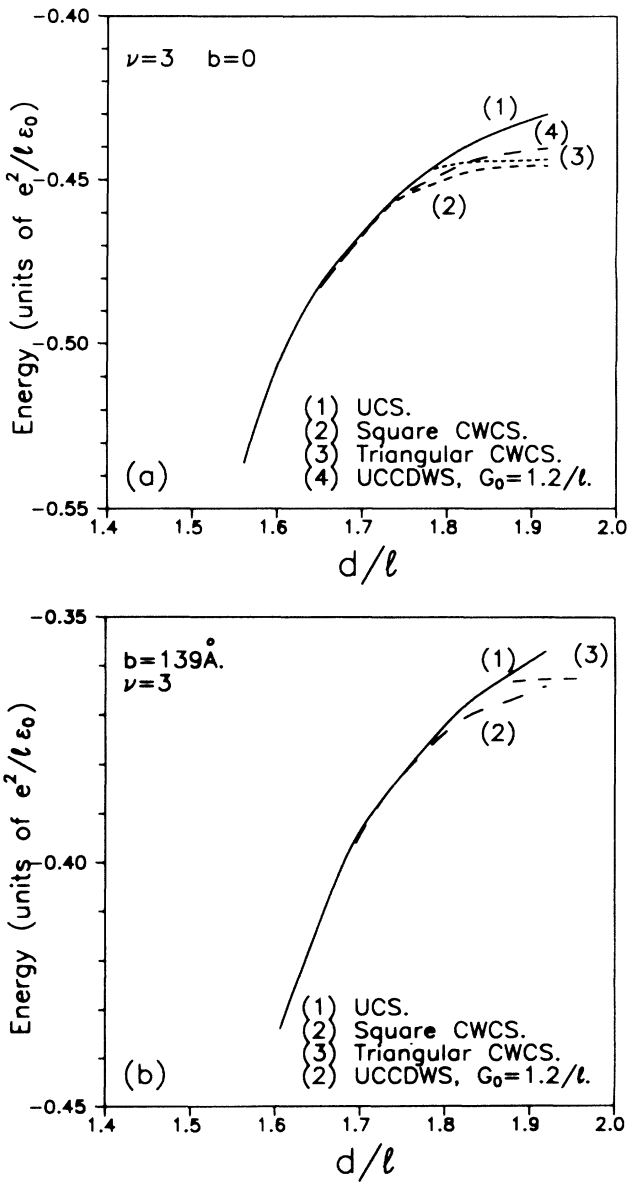

FIG. 7. Comparison of the ground-state energy as a function of the well separation of the UCS, square CWCS, triangular CWCS and UCCDWS at filling factor $\nu=3$ for (a) $b=0$ and (b) $b=139$ Å.

tion of the magnetic field. It is thus possible to compute the ground-state energy at filling factor $\nu=1$. Figures 7(a) and 7(b) show the calculated ground-state energies for the different states considered in Fig. 6 in the case of $\nu=3$ and with $b=0$ or 139 Å. (The zero of energy is different in this case.) As we can see, the situation at $\nu=3$ is qualitatively the same as that for $\nu=1$.

The above figures with tunneling were calculated assuming an areal density corresponding to that of sample 1 or 2 (we consider that these samples have approximately the same density). Comparing with Fig. 6(b), we see that the value of d (in units of l) of these two samples at $\nu=1$ is such that, according to the HFA, they should be in the CWCS. The QHE plateaus will thus be destroyed in these samples. For sample 3, Fig. 6(b) must be recalculated using a different density. We have done this and found that the ground state of this sample corresponds to a CWCS with $\langle\rho_{12}(0)\rangle=0.499\,99$. For this value of $\langle\rho_{12}(0)\rangle$, we expect that the system present a SAS gap in the excitation spectrum and this is the reason why the quantum Hall effect is observed in this sample.

Similarly, Fig. 7(b) was calculated for the density corresponding to samples 1 and 2 and we recalculated the ground-state energy for the density of sample 3. At this filling factor, the coherent inhomogeneous state exists for a small range of d only. Samples 1 and 3 are located in the region where the ground state corresponds to the UCS and thus will exhibit the QHE. On the contrary, sample 2 is in the ordered phase and will not.

VI. CONCLUSION

Working in the Hartree-Fock approximation, we have calculated the energy of different broken-symmetry ground states of the two-dimensional electron gas in a double-quantum-well system. The *transition* from homogeneous states (where the QHE is possible and interlayer coherence is maintained) to inhomogeneous states (where the QHE is not possible and interlayer coherence is lost) at a critical well separation is consistent with experiments[11] and with previous theoretical studies.[7,8] Although the study of the transition from the homogeneous phase to the CDW and WC states is interesting in itself, we want to be careful in identifying the state of the system above the critical separation with the inhomogeneous states studied in this paper. This inhomogeneity is created in order to strengthen the intrawell correlations and at a cost in interwell correlations. In the Hartree-Fock approximation studied here, the electronic ground state is a single Slater determinant and the intrawell correlations must be static, leading to inhomogeneity. It is our expectation that these inhomogeneous states are likely to be pre-empted for total filling factors larger than $\nu\sim0.5$ by homogeneous states in which the strong intralayer correlations are dynamic.[19] Aside from the absence of broken translational symmetry, we expect the properties of these ground states to be very similar to those of the Hartree-Fock ground states. A comparison between these two types of ground states asks for further studies of the transport properties of the CWCS in the DQWS.[24] Such studies are also needed in order to evaluate the stability of the different possible ground states studied in this paper. One must be aware of the limitations of the HFA studied here before comparing HF ground states with more complex homogeneous states.[19] For example, in the case of $\nu=1$, the situation for infinitely separated layers (corresponding to two noninteracting electron gases with $\nu=\frac{1}{2}$) is still a subject of controversy; at other filling factors near $\nu=1$, homogeneous states are expected in the infinite separation limit. Also, some experiments[25,26] suggest the reappearance of a fractional quantum Hall effect of a different character for the $\nu=1$ state at large well separation d, a phenomenon that clearly cannot be explained in the context of the HFA as presented here.

Note added. After this work was completed we learned of some closely related calculations by Chen and Quinn.[27]

ACKNOWLEDGMENTS

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