Wigner Crystallization in the Fractional Quantum Hall Regime: A Variational Quantum Monte Carlo Study

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(Received 25 September 1992)

Using a variational quantum Monte Carlo method, we study the two-dimensional Wigner crystal induced by a strong magnetic field in the fractional quantum Hall effect regime. Effects of exchange, intra-Landau-level correlation, and inter-Landau-level mixing on the total energy and their dependence on the carrier mass and magnetic field strength are calculated. Our results support that the recently observed reentrant behavior to an insulating phase around $\nu=\frac{1}{3}$ in p-doped GaAs/AlGaAs is a consequence of an increased stability of the Wigner crystal due to the effects of Landau-level mixing.

PACS numbers: 71.45.Nt, 73.40.Kp

Recently there has accumulated a large body of suggestive evidence for the observation of a magnetic-field-induced Wigner crystal (WC) in the fractional quantum Hall effect (FQHE) regime [1–5]. However, definitive evidence for the existence of this long-sought-after electron solid is still lacking [2,4]. Almost all of these experiments are done with n-doped samples, in which carriers have a small mass of $m^*\sim 0.07m_e$ [2–4]. With details varying, it appears clear from these experiments that there is a reentrant insulating-FQHE-insulating behavior around $\nu_c=\frac{1}{5}$ in these two-dimensional electron systems [2,4]. The only exception is one experiment performed on a low-disorder 2D hole system at the GaAs/AlGaAs interface [5]. At about the same carrier density, a reentrant behavior [5] very similar to that in the 2D electron systems is observed, but now around $\nu_c=\frac{1}{3}$. This change in ν_c was speculated by the authors [5] to be due to the effects of Landau-level (LL) mixing, being much larger in the hole system.

Theoretical estimates of the critical filling factor ν_c for the liquid-solid transition can be obtained by comparing the energies of the FQHE liquid and the WC solid. It would be a stringent consistency check of the interpretations of the above interesting experiments [2–5] if an energetic calculation could show the changes in ν_c in these different samples as they are observed experimentally. The aim of the present work is to calculate accurately the energy of the WC in various experimentally relevant situations using a variational quantum Monte Carlo (VQMC) method. In doing so, we also obtain a quantitative understanding of the roles played by exchange, intra-Landau-level correlation, and inter-Landau-level mixing in a WC. Special attention is paid to the interplay between these effects and the experimental parameters: the carrier density, carrier mass, and the strength of the magnetic field. From our calculations, we find that the effects of Landau-level mixing are indeed large enough to account for the observed difference in ν_c between the electron and the hole GaAs/AlGaAs systems [6].

2D electron/hole systems in a strong perpendicular B field exhibit a rich variety of phenomena [7]. By varying the carrier density, the carrier effective mass, and the field strength, a very intricate phase diagram is expected. Exchange-correlation effects in these systems are fundamentally affected by the presence of the magnetic field. For example, at fractional filling factors, particles can, and prefer to, correlate with each other to lower the interaction energy at no cost to the kinetic energy. There have been many studies on B-field-induced Wigner crystals in 2D [7–11]. Most of these were carried out within the Hartree-Fock approximation. With few exceptions [11], only the lowest Landau level is considered.

We now describe in some detail our VQMC calculations. In atomic units the exact Hamiltonian is given by

$$H=\sum_i \frac{[\mathbf{p}_i+\mathbf{A}(\mathbf{r}_i)]^2}{2m^*}+\frac{1}{2\varepsilon}\sum_{j\neq i}\frac{1}{r_{ij}}. \quad (1)$$

Here $\mathbf{A}$ is the vector potential, m^* is the effective mass of the carrier, and ε is the dielectric constant. In the symmetric gauge, $\mathbf{A}=(-yB/2, xB/2)$ with $\mathbf{B}$ in the $+z$ direction. We use a finite simulation cell with modified periodic boundary conditions [12]. Because of the aperiodic vector potential $\mathbf{A}$ in the Hamiltonian, only rational fields can be studied with the modified periodic boundary conditions. As a result, only the rational Landau-level filling factors are accessible in our calculations. In practice this poses no real restriction since the FQHE states, which we wish to compare our WC energies to, can only exist at some of the rational filling factors [7,10]. Calculations are carried out for a simulation cell with 100 spin-aligned electrons. Only the hexagonal lattice is considered. Calculations with different sized simulation cells show that the resulting finite-size effects are smaller than the statistical noise in our results.

The variational quantum Monte Carlo method has proven to be an accurate method in studying various condensed matter systems [13]. The present work is, to our knowledge, the first application of this method in conjunction with the periodic boundary condition in the

FQHE context. Various trial wave functions are constructed and examined to study the effects of exchange, intra-Landau-level correlation, and Landau-level mixing. The wave functions all employ one-particle orbitals of the following form which corresponds to Gaussians localized on the hexagonal lattice sites (R_j^x, R_j^y) within the simulation cell $\mathbf{L}_x \times \mathbf{L}_y$:

$$\phi_j(\mathbf{r}) = \frac{1}{\sqrt{2\pi}} \frac{\beta}{l_B} \sum_{\mathbf{T}} \exp\left\{ -\frac{\beta^2}{4l_B^2}(\mathbf{r}-\mathbf{R}_j-\mathbf{T})^2 + \frac{i}{2l_B^2}[\mathbf{r}\times\mathbf{R}_j + \mathbf{r}\times\mathbf{T} + \mathbf{R}_j\times\mathbf{T}]_z \right\}. \tag{2}$$

Here $\mathbf{T}$'s are given by $n_x\mathbf{L}_x + n_y\mathbf{L}_y$ with arbitrary integers n_x and n_y. $l_B = \sqrt{\hbar c/eB}$ is the magnetic length. β is a variational parameter to be optimized. For $\beta = 1$, $\phi(\mathbf{r})$ is solely composed of lowest Landau-level orbitals.

To make contact with earlier calculations and to establish the validity of the present variational Monte Carlo method, we first briefly summarize the results for the "Hartree," exchange-only, and correlation-only trial wave functions within the lowest Landau-level approximation. Our Hartree results are obtained for a trial wave function that is simply a product of the one-particle orbitals in Eq. (2) with $\beta = 1$. They can be evaluated exactly by the Ewald summation technique. In the exchange-only calculation with no Landau-level mixing, a trial wave function in the form of a Slater determinant, composed of the same one-particle orbitals as in the Hartree case, is used. The lowest Landau-level-correlated wave function [9] is for distinguishable particles correlated by the magnetophonons. Our derivation [14] for the magnetophonon wave function is slightly different from Lam and Girvin's original work [9]. The final form of the correlated wave function $\psi_{\rm cor}$ in the large B-field limit is, however, the same:

$$\psi_{\rm cor} = \exp\left[\frac{1}{4l_B^2} \sum_{i,j} \xi_i B_{ij} \xi_j \right] \prod_i \phi_i(\mathbf{r}_i). \tag{3}$$

Here ϕ_i's are the single-particle orbitals in Eq. (2). ξ_i is the deviation of the ith electron from its lattice site R_i in complex coordinates. The B_{ij}'s give rise to the correlation effects. Its Fourier transform $B(\mathbf{k})$ can be written as

$$B(\mathbf{k}) = e^{i\theta_{\mathbf{k}}} \frac{\omega_L^0(\mathbf{k}) - \omega_T^0(\mathbf{k})}{\omega_L^0(\mathbf{k}) + \omega_T^0(\mathbf{k})}, \tag{4}$$

where

$$\cos\theta_{\mathbf{k}} = -\frac{(A-B)/2}{[(A-B)^2/4 + C^2]^{1/2}}, \qquad \sin\theta_{\mathbf{k}} = -\frac{C}{[(A-B)^2/4 + C^2]^{1/2}}. \tag{5}$$

Here A and B are the diagonal elements of the dynamical matrix at $\mathbf{k}$ for the hexagonal WC lattice with no magnetic field. C is the off-diagonal element. The ω_T^0 and ω_L^0 are, respectively, the transverse and longitudinal phonon frequencies.

The energies from the Hartree, exchange-only, and correlation-only calculations, all of which are within the lowest Landau-level approximation, are given in Table I. The comparison of Hartree and exchange-only results gives the size of "bare" exchange energy. In principle, one can antisymmetrize the wave function of Eq. (3) and obtain an estimate of the exchange energy that is "screened" by the magnetophonon correlations. In practice it is difficult to carry out such a scheme with the variational Monte Carlo method because the wave function resulting from this explicit antisymmetrization is no longer in the Jastrow-Slater form. However, the upper bound for the exchange energy, set by the bare exchange interaction, is already very small for $\nu \leq \frac{1}{3}$. The energy gain from antisymmetrizing Eq. (3) will be even smaller. Landau-level mixing decreases the exchange overlap still further. We shall come back to this point later.

Previous Hartree-Fock calculations [8] are mostly done for a charge-density-wave (CDW) state that is in principle not necessarily the same as our explicit WC state. But as we see from Table I, the resultant energies are virtually identical. Our energies for the correlation-only calculation are the same as those obtained by Lam and Girvin [9] using a special k-point sampling method. Taking the fractional quantum Hall liquid energies from Ref. [10] that were obtained using the Laughlin wave function which is also within the lowest Landau-level approximation, the crossover from the liquid to solid is $\nu_c \sim 1/6.5$, as

TABLE I. Energies (in effective atomic units) of the hexagonal Wigner crystal from various lowest LL only calculations at $r_s = 1.784$. A constant kinetic energy $\frac{1}{2}\hbar\omega_C$ is subtracted. All energies at other r_s's may be obtained by simply scaling by $1/r_s$.

		Exchange only		Correlation only		Laughlin
ν	Hartree	Present	Ref. [7]	Present	Ref. [8]	Ref. [9]
$\frac{1}{2}$	−0.4733	−0.4972(3)	−0.4976	−0.4929(13)	−0.4928	
$\frac{1}{3}$	−0.5294	−0.5338(8)	−0.5334	−0.5419(9)	−0.5422	−0.5631
$\frac{1}{4}$	−0.5561	−0.5567(5)	−0.5557	−0.5650(3)	−0.5643	
$\frac{1}{5}$	−0.5706	−0.5707(1)	−0.5706	−0.5779(3)	−0.5775	−0.5807
$\frac{1}{7}$	−0.5859	−0.5858(1)	−0.5852	−0.5910(1)	−0.5901	−0.5893

found by Lam and Girvin [9].

Motivated by the recent experiment on 2D hole systems [5], we now concentrate on the effects of Landau-level mixing. There are two independent variables in considering the energetics: the filling factor ν (determined by the carrier density and the magnetic field) and the electron gas parameter r_s (determined by the density and the effective mass). The two relevant energies are the inter-Landau-level spacing $\hbar\omega_C$ and the Coulomb interaction $E_c = e^2/\epsilon d$ where $\pi d^2 = 1/n$. They are related as follows:

$$E_c/\hbar\omega_C = \nu r_s/2 . \quad (6)$$

The ratio is related to the amount of Landau-level mixing. The r_s in the above equation is measured in the effective atomic units. It takes the value of $r_s \sim 2$ for typical 2D electron systems. But for the 2D hole system investigated it is $r_s \sim 25$, if one assumes an effective mass $m^* \sim 0.6m_e$ [15]. If $m^* \sim 0.3m_e$, r_s would be ~ 13 [5]. Our calculations are carried out for $r_s = 2$ and 20. Calculations ignoring Landau-level mixing may be regarded as for the extreme case of $r_s = 0$, corresponding to the high density, small mass limit. It is not surprising that this ceases to be a good approximation for the case of 2D hole systems where νr_s approaches 10.

To mix in higher Landau levels into the ground-state wave function is to lower the interaction energy at the cost of kinetic energy. The rigorous lower bound of the interaction energy is given by that of point-charge particles sitting at the lattice sites, i.e., the classical Ewald energy. In the presence of strong Coulomb repulsion between neighboring electrons, it is energetically favorable to have (1) a charge-density distribution more localized at the lattice sites than that given by the lowest Landau-level orbitals, and (2) a nonanalytic correlation term in the Jastrow factor which optimizes the dynamical short-range avoidance between electrons. Based on these physical considerations, we have allowed β in Eq. (2) to vary and have introduced an additional correlation factor between particles $\mathbf{r}_i$ and $\mathbf{r}_j$ [14,16] to the exponent of the correlation part of the wave function in Eq. (3): $u(r = |\mathbf{r}_i - \mathbf{r}_j|) = (A/\sqrt{r})[1 - \exp(-\sqrt{r/F} - r/2F)]$. ($A$ and F are variational parameters.) We evaluated the consequent kinetic energy and interaction energy until an optimal energy is reached.

Significant lowering in energy due to Landau-level mixing is obtained with just the wave function form given by Eq. (3) with the one-particle orbital Gaussians scaled by β. We have varied both the Gaussian size and the overall coefficient of the magnetophonon correlation term in the Jastrow factor in Eq. (3). The latter is found to have little effect on the energy [14]. In Fig. 1, we show the total energy as a function of β for $r_s = 20$ and 2 at $\nu = \frac{1}{3}$. We find an increase in density at the lattice sites by $\delta\rho(0)/\rho(0) = 70\%$ and a lowering in energy by $\delta E/(E - \frac{1}{2}\hbar\omega_C) = -4.4\%$ at $r_s = 20$. They are, respectively, 10% and -0.8% at $r_s = 2$.

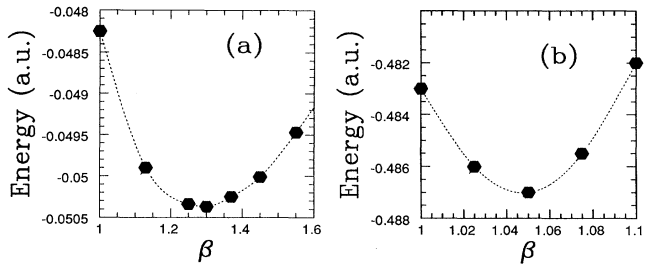

FIG. 1. (a) $E^{\text{total}} - \frac{1}{2}\hbar\omega_C$ (per electron) vs β for $\nu = \frac{1}{3}$ at $r_s = 20$. (b) Same as (a) for $r_s = 2$. Energies are in the effective atomic unit. Statistical noise is given by the size of the data points.

To appreciate the importance of the 4% lowering in energy, we note that the interaction energy of the lowest Landau-level Lam-Girvin wave function is only 12% higher than the absolute minimum given by the Ewald energy. At $r_s = 20$, this difference is reduced by $\frac{1}{3}$ from allowing the Landau levels to mix. In comparison, the bare exchange at $\nu = \frac{1}{3}$, i.e., the difference between the Hartree and exchange-only results, is only 0.8%. Further, at $r_s = 20$, a 30% reduction in the extent of the one-particle orbitals from Landau-level mixing and the screening movements due to the magnetophonon correlation factor render the final exchange energy negligible compared to the correlation and Landau-level mixing effects.

Additional lowering in energy is achieved with the Landau-level mixing Jastrow factor. Our final results are obtained with both Landau-level mixing mechanisms included. Calculations are carried out at $\nu = \frac{1}{2}$, $\frac{1}{3}$, $\frac{1}{5}$, and $\frac{1}{7}$ for $r_s = 2$ and 20. Results for $r_s = 20$ are plotted in Fig. 2, where we show the energy for the case of exchange-only with no Landau-level mixing, the case of correlated wave function with no Landau-level mixing, and finally the case of the correlated wave function with Landau-level mixing. The energy of the incompressible FQHE liquid [10] based on Laughlin's variational wave function is also shown for filling factors $\frac{1}{3}$, $\frac{1}{5}$, and $\frac{1}{7}$. The line passing through the three liquid points is a spline fit to the data. It does not show the cusps that must occur at filling factors where the FQHE states exist. Also shown in Fig. 2 are the energies of the FQHE states at $\frac{1}{3}$, $\frac{1}{5}$, and $\frac{1}{7}$ with Landau-level mixing, according to the recent calculations by Price, Platzman, and He [16]. The details of the phase diagram will be affected by temperature and disorder, both of which favor the Wigner crystal phase.

At $r_s = 20$, our calculated energy curve for the WC phase lies entirely below the Laughlin wave function energies for $\nu \leq \frac{1}{3}$. We note that, as seen in Fig. 2, Landau-level mixing effects are in fact larger than those of intralevel exchange-correlation effects in this case [5]. We expect that Landau-level mixing effects will be smaller in the liquid phase. In the solid phase, both Hartree and correlation energies can be lowered by allowing

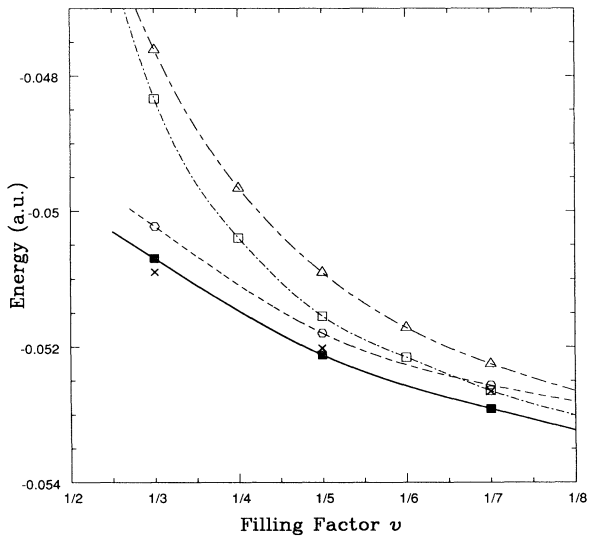

FIG. 2. $E^{\text{total}} - \frac{1}{2}\hbar\omega_C$ of the WC at $r_s = 20$ compared with those of the FQHE liquid. Energies are in the effective atomic unit. (Δ)—WC with exchange only and no Landau-level mixing. (□)—WC with correlation but no Landau-level mixing. (■)—Correlated WC with Landau-level mixing. (○)—Laughlin state with no Landau-level mixing from Ref. [10]. (×)—Laughlin state with Landau-level mixing from Ref. [16].

Landau-level mixing. From our calculations, the former appears to be the main mechanism for lowering the energy. But this mechanism is entirely lost in the liquid phase where any lowering in the interaction energy must come from making the pair-correlation function more repulsive: Being a uniform state the liquid Hartree energy will not be altered by Landau-level mixing. The work of Price, Platzman, and He [16] on the effects of Landau-level mixing in the FQHE state shows that the lowering in the liquid energy is indeed substantially smaller than that in the solid: for $r_s = 20$ at $\nu = \frac{1}{3}$, lowering in energy from Landau-level mixing for the FQHE liquid state is only $\frac{1}{4}$ of that which we find for the WC solid (see Fig. 2). As a result, for $r_s = 20$, the FQHE state is only slightly more stable than the WC state at $\nu = \frac{1}{3}$ for a pure system with no disorder. The WC becomes lower in energy at $\nu = \frac{1}{5}$. For $r_s = 2$, however, the WC state is higher in energy at $\nu = \frac{1}{5}$ but remains lower in energy at $\nu = \frac{1}{7}$ than the FQHE state.

In summary, we have carried out the first variational quantum Monte Carlo calculations for the B-field-induced Wigner crystal phase in 2D. We take into account both the short-range and long-range correlation effects in the WC and provide a rigorous variational upper bound for the WC energy. Landau-level mixing effects are shown to be significant in the range of carrier density, effective mass, and strength of the magnetic field of experimental interest. Our results show that these effects are most likely to be responsible for the change from a 2D electron system to a 2D hole system in the critical filling factor ν_c, around which a reentrant insulating-FQHE-insulating behavior has been observed. Taking the calculations and the experiments together, there are now good reasons to believe that the insulating phases around the FQHE states at ν_c are Wigner crystals pinned by impurity potential.

We acknowledge communications with Rod Price and Phil Platzman concerning some of their unpublished results. We also thank Pui Lam for the timely replies to several of our questions. This work was supported by NSF Grant No. DMR91-20269 and by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. X.Z. thanks the Center for Advanced Materials for its support. CRAY computer time was provided by the NSF at the San Diego Supercomputing Center and by the Department of Energy.

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