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Liquid-solid transition and the fractional quantum-Hall effect

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The critical Landau-level filling factor ν_c for the transition from Laughlin's liquid state to a Wigner crystal is determined by comparing the energies of these states. The Wigner-crystal energy is substantially improved over the Hartree-Fock result by using a variational wave function which includes particle correlations. The liquid-state energy is obtained from the Monte Carlo calculation of Levesque, Weis, and MacDonald. We find ν_c to be slightly larger than $\frac{1}{7}$ which is consistent with the experimental observation by Mendez and co-workers that the fractional quantum-Hall effect does not occur for $\nu \leq \frac{1}{7}$. The improvement in the crystal energy by correlation is essential to this agreement since without correlations, $\nu_c \sim \frac{1}{10}$. In addition the crystal correlation energy explains the very low temperatures required to see the $\nu = \frac{1}{5}$ liquid state.

The discovery of the fractional quantum-Hall effect[1,2] (FQHE) has brought considerable interest[3-16,20] to the following question: what is the nature of the ground state of a two-dimensional interacting electron system at very high magnetic fields? At low density (small Landau-level filling factor ν) the ground state is expected to be a Wigner crystal (WC).[3-5,17] At moderate density ($\nu = \frac{1}{3}, \frac{1}{5}$) a special incompressible liquid state proposed by Laughlin[9] has an energy lower than the WC. One, therefore, anticipates a liquid-solid transition at some intermediate filling ν_c. Since the WC has gapless excitations (phonons) an immediate experimental consequence of this transition is that the FQHE will not be observed for $\nu < \nu_c$.

Several developments have occurred recently which now make a realistic estimate of ν_c possible as well as timely. On the experimental front, Mendez and co-workers[18,19] have obtained indirect evidence that ν_c may be $\frac{1}{7}$ or larger. They have found in high-mobility GaAs samples that the FQHE does not occur for $\nu < \frac{1}{5}$ and suggest that Wigner crystallization may be the cause. On the theoretical front, accurate liquid-state energies for a wide range of ν have recently been calculated by Levesque, Weis, and MacDonald.[20] These essentially exact Monte Carlo results lie significantly above the values obtained by Laughlin using the hypernetted-chain approximation.[9] Using the Hartree-Fock (HF) energy for the crystal and their Monte Carlo values for the liquid-state energy, Levesque *et al.*,[20] obtained $\nu_c \sim \frac{1}{10}$.

The WC energy has until now only been computed within the HF approximation[3-5,20] which neglects correlations. We have directly calculated the WC ground-state energy using a variational wave function which includes particle correlations. This wave function is related to that recently proposed by Maki and Zotos[5] but is multiplied by a correlation-factor. This factor is chosen to be a Gaussian so that evaluation of the energy is still relatively simple. We find that correlations reduce the WC energy below the HF value by $4\times 10^{-3} e^2/\epsilon l$ (where ϵ is the dielectric constant and l the magnetic length) at $\nu = \frac{1}{5}$, an effect several times larger than that estimated from second-order perturbation theory.[4] Using our improved WC energies and the liquid-state energies of Levesque *et al.*,[20] we obtain the liquid-solid transition at ν_c slightly greater than $\frac{1}{7}$ in good agreement with the recent experimental observations of Mendez and co-workers.[18,19]

In this Rapid Communication we will briefly discuss our variational wave function and the procedure for evaluating the ground-state energy. Comparison with experiment will then be made. A more detailed discussion of the wave function and the numerical calculation will be presented in a longer paper. Except where otherwise noted we will use units such that $l = e^2/\epsilon l = 1$ throughout. For compactness of notation, both complex numbers and vectors will be used to represent particle coordinates in the two-dimensional space, e.g., the complex number $z = x + iy$ is related to the vector $\vec{z} = (x,y)$. Since Laughlin's liquid-state wave function was chosen to be entirely within the lowest spin state of the lowest Landau level, we will make the same restriction on our variational wave function to ensure a consistent comparison. In any case, this assumption has been shown to be valid in the magnetic field regime of interest.[4,21]

Maki and Zotos[5] have proposed the following wave function to describe an uncorrelated Wigner crystal (UWC)

$$\psi^u[z] = A\, \Pi_l\, \phi_{R_l}(z_l), \qquad (1)$$

where A is the antisymmetry operator and $\phi_{R_l}(z_l)$ a single-particle state localized at a site R_l on a triangular lattice and is given by

$$\phi_{R_l}(z_l) = (2\pi)^{-1/2} \times \exp[-\tfrac{1}{4}|z_l - R_l|^2 - \tfrac{1}{4}(z_l^* R_l - z_l R_l^*)] \; . \qquad (2)$$

Using this ansatz for the wave function, Maki and Zotos obtained essentially the same results as the HF calculation.[3,4] The wave function given by Eq. (1) has its largest amplitude when the particles are at the equilibrium lattice sites R_l and decreases for fluctuations, $\xi_l = z_l - R_l$ away from these sites. Because ψ^u is a single Slater determinant, there are no correlations between these fluctuations.

The Coulomb energy can be lowered by correlating the fluctutions in particle positions in such a way that energetically favorable fluctuations are given large amplitudes while unfavorable fluctuations are given small amplitudes. To accomplish this we write our variational wave function for a correlated Wigner crystal (CWC) as

$$\psi^c[z_i] = \exp\left(\tfrac{1}{4} \sum_{ij} \xi_i B_{ij} \xi_j\right) \prod_i \phi_{R_i}(z_i) \quad , \tag{3}$$

where the B_{ij} are (complex) variational parameters which determine the correlations and B_{ij} is a shorthand notation for

$$B_{ij} = B(\vec{R}_i, \vec{R}_j) = B(\vec{R}_i - \vec{R}_j). \tag{4}$$

The last equality follows from the lattice translational symmetry. We have dropped the antisymmetry operator because we have found that exchange is negligible for $\nu < \frac{1}{3}$ (due to the rapid falloff of the Gaussian wave function) and this greatly simplifies the calculation.

The quantity to be minimized for N particles is

$$E = \frac{1}{2N} \sum_{i \neq j} \left\langle \psi^c \middle| \frac{1}{|z_i - z_j|} \middle| \psi^c \right\rangle \Big/ \langle \psi^c | \psi^c \rangle \quad . \tag{5}$$

The kinetic energy contributes an irrelevant constant to E since ψ^c contains only states from the lowest Landau level. Since it is a nontrivial numerical problem to find the optimal set $\{B_{ij}\}$ which minimizes E, we adopt the following strategy. We first expand the Coulomb potential to second order in the fluctuations ξ_i. Within the harmonic approximation it is possible to obtain analytically the optimum $\{B_{ij}\}$. We then use the resulting variational wave function ψ^c to evaluate E in Eq. (5) exactly (i.e., without making the harmonic approximation). Hence, this procedure yields a rigorous variational bound on the energy. One can show *a posteriori* that this procedure yields a nearly optimum bound on the energy since the anharmonic contributions to the energy turn out to be very small. This is reasonable since at least for small ν, the fluctuations ξ_i which are of the order of the magnetic length are much smaller than the nearest neighbor distance.

In the harmonic approximation the optimal $\{B_{ij}\}$ are related to the phonon frequencies of the classical (point charge) Wigner crystal. We define

$$B(\vec{q}) = \sum_{\vec{R}} e^{-i\vec{q} \cdot \vec{R}} B(\vec{R}) \equiv B_q e^{i\theta_q} \quad , \tag{6}$$

where $\vec{q} = (q_x, q_y)$ is a vector in the Brillouin zone. We find that the optimal $B(\vec{q})$ is given by

$$B_q = \frac{\omega_L(\vec{q}) - \omega_T(\vec{q})}{\omega_L(\vec{q}) + \omega_T(\vec{q})} \quad , \tag{7}$$

where $\omega_L(\vec{q})$ and $\omega_T(\vec{q})$ are the longitudinal and transverse classical phonon frequencies, respectively, and θ_q in Eq. (6) is a phase related to the classical dynamical matrix. The reason that B_q is related to the phonon frequencies is that the fluctuations ξ_i can be expanded in terms of the phonon eigenmodes of the classical point-charge Wigner crystal. The correlations induced by the $B(\vec{q})$ lower the energy by favoring fluctuations which correspond to transverse modes and disfavoring fluctuations corresponding to longitudinal modes.

The energy per particle for the CWC given by Eq. (5) was evaluated numerically using the $B(\vec{q})$ given by Eqs. (6)–(7). For $\nu \leqslant \frac{1}{2}$ the result can be expressed as

$$E^c_{\mathrm{WC}} = -0.782\,133\nu^{1/2} + 0.2410\nu^{3/2} + 0.16\nu^{5/2} \quad . \tag{8}$$

The first term corresponds to the classical energy[22] and the remaining terms correspond to the harmonic and quartic expansion of the Coulomb potential. The coefficients of the first and second terms can be evaluated as accurately as desired. Only the coefficient of the last term is obtained by fitting Eq. (8) to the calculated energies. The error in this fitting does not exceed 10^{-3}. The Hartree-Fock WC energy for $\nu \leqslant \frac{1}{2}$ can be represented by

$$E^{\mathrm{HF}}_{\mathrm{WC}} = -0.782\,133\nu^{1/2} + 0.2823\nu^{3/2} + 0.18\nu^{5/2} - 1.41e^{-2.07/\nu} \quad . \tag{9}$$

The first three terms have the same meaning as in Eq. (8) and the last term approximates the exchange. This expression is somewhat more accurate than the form chosen by Levesque *et al.*[20] Laughlin's liquid state[9] with filling factor $\nu = 1/m$ where m is an odd integer has an energy accurately given by the interpolation formula of Levesque *et al.*[20]

$$E_L = -0.782\,133\nu^{1/2} + 0.165\nu^{1.24} - 0.009\nu^{2.2} \quad . \tag{10}$$

Table I presents a comparison between the CWC, the Hartree-Fock WC, and the liquid-state energies for $\nu = \frac{1}{3}$, $\frac{1}{5}$, and $\frac{1}{7}$.

TABLE I. Comparison between the Wigner-crystal energy and the liquid-state energy at $\nu = \frac{1}{3}$, $\frac{1}{5}$, and $\frac{1}{7}$. The liquid-state energy E^a_L is from the Monte Carlo calculation of Levesque *et al.* (Ref. 20) and E^b_L is from the hypernetted-chain approximation of Laughlin (Ref. 9). The crystal energy is from the present calculation. Energies are in units of $e^2/\epsilon l$. Numerical accuracies quoted from the references are indicated in parentheses.

		ν	
	$\frac{1}{3}$	$\frac{1}{5}$	$\frac{1}{7}$
$E^{\mathrm{HF}}_{\mathrm{WC}}$	-0.3885 $(\pm < 10^{-4})$	-0.3219 $(\pm < 10^{-4})$	-0.2794 $(\pm < 10^{-4})$
E^c_{WC}	-0.3948 $(\pm\ 0.0005)$	-0.3258 (± 0.0005)	-0.2816 (± 0.0005)
E^a_L	-0.4100 $(\pm\ 0.0001)$	-0.3277 (± 0.0002)	-0.2810 (± 0.0002)
E^b_L	-0.4156 (± 0.0012)	-0.3340 (± 0.0028)	

Experimentally[1,2,18,19] the filling factor is varied by changing the magnetic field at fixed electron density (in GaAs-AlGaAs systems). In Fig. 1 we plot E^{C}_{WC}, E^{HF}_{WC}, and E_L referenced to the classical energy as a function of magnetic field for a typical density of $n = 10^{11}/\mathrm{cm}^2$ and dielectric constant $\epsilon = 13$. Energies are here expressed in kelvins.

At $\nu = \frac{1}{2}$ E^{C}_{WC} is slightly greater than E^{HF}_{WC} because exchange has not been included in E^{C}_{WC}; however, for $\nu < \frac{1}{3}$ exchange is negligible and correlation dominates. The crossover between the (interpolated) liquid energy and the WC energy occurs at $1/\nu_c = 6.5 \pm 0.5$. This crossover point is in agreement with the experimental results of Mendez and co-workers.[18,19] They searched for the FQHE in high-mobility GaAs samples at temperatures of 0.5 and 0.068 K. No effect was observed for $\nu < \frac{1}{5}$ suggesting that Wigner crystallization has occurred. At $\nu = \frac{1}{5}$ a broad structure in ρ_{xx} consistent with the FQHE was observed but only at the lower temperature. Our calculations show $E^{C}_{WC} - E_L \simeq 0.3$ K at $\nu = \frac{1}{5}$ (for the electron density of their sample, $n = 6 \times 10^{10}/\mathrm{cm}^2$) which seems to be consistent with the absence of the FQHE at 0.5 K. Improvement on the WC energy by correlation is essential to the agreement between theory and experiment since without correlation the liquid-solid transition point would have been at $\nu_c \sim \frac{1}{10}$ and furthermore $E^{HF}_{WC} - E_L \simeq 1$ K at $\nu = \frac{1}{5}$.

Several caveats are in order. We have treated here only the zero-temperature limit. A second point is that because of the finite extent of the electron wave functions in the direction normal to the plane of the inversion layer the effective Coulomb potential deviates from $1/r$ at small distances. MacDonald and Aers[23] have estimated the corrections to ν_c due to this effect and found them to be negligible. For the purpose of consistent comparison with the liquid-state energies we have neglected Landau-level mixing but this appears to be a good approximation.[4,21] Finally we note that we have neglected possible effects due to the small but nonzero static disorder in the samples.

In conclusion, we have determined the liquid-solid transition point of a two-dimensional electron gas in a quantizing magnetic field by comparing accurate variational estimates of the ground-state energies of the liquid and solid states. Our theoretical results for the critical density and the relevant energy scales are in good agreement with the presently available experimental data. Correlation effects which were previously believed to be relatively unimportant for the Wigner crystal were shown here to be significant and in fact essential to reconcile theory and experiment. We believe that these results represent strong indirect evidence for Wigner-crystal formation at filling factor $\nu < \frac{1}{5}$. Experiments attempting to directly observe this phenomenon would be of great interest.

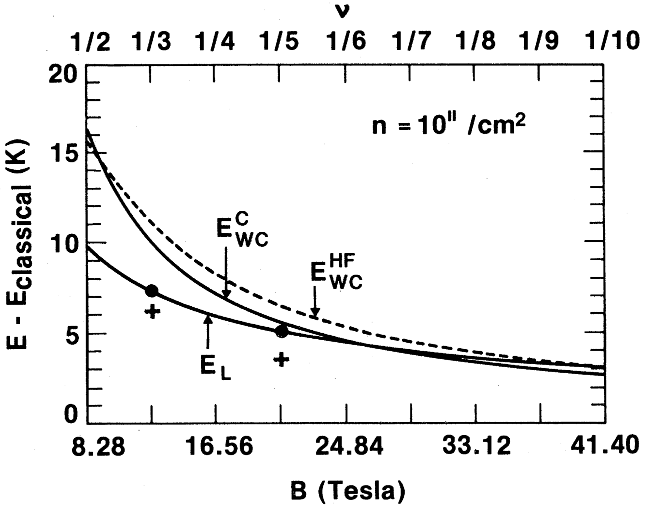

FIG. 1. Energy per electron vs magnetic field strength at a fixed electron areal density, $n = 10^{11}/\mathrm{cm}^2$. The upper horizontal axis shows the corresponding Landau-level filling factor. The energies are referenced to the classical Wigner-crystal energy and measured in units of equivalent temperature in kelvins. The curves E^{HF}_{WC} and E^{C}_{WC} are the Hartree-Fock and correlated Wigner-crystal energies, respectively. The two solid circles are the liquid energies at $\nu = \frac{1}{3}$ and $\frac{1}{5}$ obtained by Monte Carlo calculations (Ref. 20) and the curve E_L is the interpolation formula given in Ref. 20. The two crosses are the liquid energies from Laughlin's hypernetted chain calculation (Ref. 9).

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