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Fractional Quantum Hall Liquid, Wigner Solid Phase Boundary at Finite Density and Magnetic Field

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At finite magnetic field and fixed filling factor ν, as the particle density decreases, the fractional quantum Hall state will at some point give way to the Wigner solid. We calculate the ground-state energy of a Laughlin-like variational wave function at finite magnetic field and density by a quantum Monte Carlo method and compare the results with a calculation of the Wigner solid energy to get an estimate of the zero temperature finite density phase boundary.

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The fractional quantum Hall effect is a remarkable macroscopic quantum phenomenon occurring in a 2D electron gas at high perpendicular magnetic fields B and low temperatures T [1]. If the 2D gas is confined in GaAs, the high mobility samples for a range of fields have an accurately quantized Hall resistivity determined only by the fractional filling of the lowest Landau level and a longitudinal resistivity which decreases exponentially as $T \to 0$.

In this regime, it is generally believed that the 2D electron gas is best described as a strongly correlated quantum liquid, the so-called Laughlin liquid (LL).

At sufficiently high fields it is also known that these same high mobility GaAs systems become resistive, i.e., the longitudinal resistivity begins to increase exponentially as $T \to 0$. The value of B at which this occurs in the best samples is a function of the dimensionless density as well as the fractional filling of the Landau level. In this regime many other types of experiments [2–7] suggest that the 2D electron system is, in fact, a pinned electron solid, the so-called Wigner solid (WS) with no gap in the excitation spectrum, except perhaps for a gap which comes about due to pinning by impurities.

For an ideal system consisting of $n = 1/\pi a^2$ carriers/cm^2 of mass m^* interacting via a Coulomb interaction screened by a static dielectric constant ϵ, the phase boundary between the LL and WS is completely characterized by three dimensionless parameters: the filling factor ν, the dimensionless density r_s, and the dimensionless temperature Γ. More precisely $\nu = 2\ell^2/a^2 \equiv 2E_F/\hbar\omega_c$ [$\ell = (\hbar c/eB)^{1/2}$, $E_F = \pi n/m^*$, and $\omega_c = eB/m^*c$], $r_s = a/a_B$ ($a_B = \epsilon\hbar^2/m^*e^2$), and $\Gamma = (e^2/\epsilon a)/k_BT$. In the regime where the density is high it is convenient to think of r_s as equivalent to a Landau-level mixing parameter $\lambda = (e^2/\epsilon a)/\hbar\omega_c \equiv \frac{1}{2}\nu r_s$.

All microscopic calculations to date of the phase boundary between LL and WS have been restricted to the $\Gamma = r_s = 0$ limit. Some reliable estimates of the solid energy were made through the use of a quadratic variational wave function for a set of distinguishable particles [8] or the use of a perturbation expansion about the energy for a harmonic solid [9]. This energy was then compared with the energy of the LL. Since the solid is almost harmonic it is possible to calculate its energy by at least two methods at arbitrary density [9, 10]. To determine the phase boundary between LL and WS it is also necessary to calculate accurately the energy of the LL as a function of density.

In this Letter we present the results of a variational Monte Carlo calculation of the energy of a fractional quantum Hall liquid at finite r_s and at $\nu = 1/3$, $1/5$, $1/7$, and $1/9$. We use a variational wave function ψ_α^ν, which is of the Laughlin form at filling factor ν, multiplied by a Jastrow factor with a single parameter α to calculate the energy. The Laughlin wave function has the minimum possible kinetic energy and it does a superb job of keeping the particles as far from one another as possible considering the limited basis set. The Jastrow factor in our new wave function introduces additional correlations which keep the electrons further apart, i.e., it makes the LL look more like a solid. The reduction of potential energy which results, however, is at the expense of additional kinetic energy, and it remains to show how much lowering of the total energy we get at any given density. We do, however, know that at large enough r_s the potential wins out and as we shall see it is possible to gain a significant amount of energy over the LL energy at experimental densities.

In the numerical calculation we place a finite number of particles N on a sphere of radius R ($n = N/4\pi R^2$). We assume that a uniform neutralizing background charge is on the surface of the sphere and that a magnetic monopole giving $2S$ magnetic flux quanta which extend radially through the surface is at the center. If $m = 1/\nu$ is an odd integer, then $2S = m(N-1)$. If we choose a as the unit of length and $e^2/2a_B\epsilon$ as the unit of energy, the Hamiltonian is

$$H = \frac{1}{r_s^2} T + \frac{2}{r_s} V - \frac{2}{r_s} N^{3/2}, \tag{1}$$

where T is the kinetic energy operator, V is the potential energy operator, and the last term is the contribution from the uniform background charge. The operator T for N particles on the sphere, in these units, is

$$T = \frac{4}{N} \left(\sum_i |\mathbf{L}_i|^2 - S^2 \right). \tag{2}$$

Here the angular momentum operator [11, 12]

$$\mathbf{L} = \mathbf{R} \times (\mathbf{p} - e\mathbf{A}) + S\hat{\mathbf{\Omega}}, \tag{3}$$

where $\mathbf{R} = R\hat{\mathbf{\Omega}}$ is a point on the surface of the sphere and the vector potential is $\mathbf{A} = -(S/R)\cot\theta\,\hat{\boldsymbol{\phi}}$.

Single-particle eigenstates in this gauge are

$$Y_{S\ell m} = M_{S\ell m} u^{S-m} v^{S+m} P_{\ell - S}^{S+m, S-m}(u\bar{u} - v\bar{v}), \qquad M_{S\ell m} = \left[\frac{2\ell + 1}{4\pi} \frac{(\ell - S)!(\ell + S)!}{(\ell - m)!(\ell + m)!} \right]^{1/2}, \tag{4}$$

where $P_n^{\alpha,\beta}(x)$ is a Jacobi polynomial and $u \equiv e^{-i\phi/2}\cos(\theta/2), v \equiv e^{i\phi/2}\sin(\theta/2)$ are convenient spinor coordinates. If we assume that the distance between particles i and j is the chord distance $r_{ij} = 2R|u_i v_j - u_j v_i|$, then

$$V = \frac{1}{\sqrt{N}} \sum_{i<j} \frac{1}{|u_i v_j - u_j v_i|}. \tag{5}$$

After experimenting with several Jastrow factors we chose a trial wave function of the form

$$\psi_\alpha^\nu = \prod_{i<j} (u_i v_j - u_j v_i)^m \exp\left(\frac{-\alpha}{|u_i v_j - u_j v_i|^{1/2}} \right). \tag{6}$$

The rather smooth Jastrow factor $-\alpha/r^{1/2}$ introduces long-range solidlike correlations and as we shall see gives us a reasonable energy lowering of the liquid as r_s increases. Although the form of the Jastrow factor is the same as Ceperley's [13], the wave function as a whole does not behave as his because of the difference in prefactors. We have obtained variational energies as a function of r_s for $\nu = 1/3$, 1/5, 1/7, and 1/9. We use the Metropolis algorithm to evaluate expectation values of the kinetic and potential energy operators T and V for various α in the state ψ_α^ν. A polynomial in α is then fitted to the data from the Monte Carlo code to give a continuous approximation to $T_\nu(\alpha) = \langle \psi_\alpha^\nu | T | \psi_\alpha^\nu \rangle$ and $V_\nu(\alpha) = \langle \psi_\alpha^\nu | V | \psi_\alpha^\nu \rangle$. The variational energy $E_\nu(r_s)$ for a given r_s and ν is then found by minimizing $E_\nu(r_s, \alpha) = (1/r_s^2)T_\nu(\alpha) + (2/r_s)V_\nu(\alpha)$.

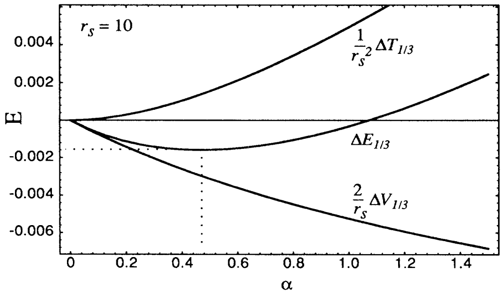

FIG. 1. Change relative to the Laughlin state in kinetic $\Delta T_{1/3}(\alpha)$, potential $\Delta V_{1/3}(\alpha)$, and total energy $\Delta E_{1/3}(r_s, \alpha)$ at $r_s = 10$, $\nu = 1/3$ as a function of the variational parameter α. The statistical error is too small to show.

A typical result is shown in Fig. 1 for $\nu = 1/3$, $r_s = 10$, and $N = 100$. The minimum is at $\alpha = 0.47$ and the energy gain ΔE relative to the Laughlin state is 0.0016. The Monte Carlo code was run until the statistical error was less than $0.001/r_s$ for $r_s < 100$. In order to evaluate finite-size effects, runs were made at $\nu = 1/3$ and 1/5 with 50, 100, and 200 particles. On the sphere, the zero-point energy $\frac{1}{2}\hbar\omega_c = (2/\nu r_s^2)(1 - 1/N)$ of the single-particle states in the lowest Landau level varies somewhat with particle number. Once this zero-point energy was subtracted from the total energy, differences in energy of $\lesssim 0.001/r_s$ were found between the energies for 50 and 100 particles and no differences within the statistical error of the Monte Carlo code were found between the energies for 100 and 200 particles. The results quoted in Table I are for systems of 100 particles at $\nu = 1/3$ and 1/5, and for systems of 50 particles at $\nu = 1/7$ and 1/9.

Figure 2 shows the pair correlation functions $g(r)$ we obtained for the $\nu = 1/3$ liquid at various r_s. As r_s increases, mixing in higher Landau levels becomes progressively less costly in energy and more correlations are introduced. The correlation hole increases in width, the first peak becomes higher, and at higher r_s other peaks begin to become apparent. At very large r_s ($r_s > 300$), the pair-correlation function becomes indistinguishable from the pair-correlation functions for a classical 2D electron crystal at some finite temperature [14].

In order to determine the value of r_s at the LL-WS transition, we need, as discussed, a rather accurate evaluation of the energy of the solid. Esfarjani [15], following

TABLE I. Coefficients for an expansion of the trial wave function liquid energy of the form $r_s(E - \hbar\omega_c/2) = a_0 + a_1 r_s + a_2 r_s^2 + a_3 r_s^3$. The error in fitting is less than $0.001/r_s$ for $r_s < 100$ at $\nu = 1/3$ and 1/5, and for $r_s < 20$ at $\nu = 1/7$ and 1/9.

ν	a_0	$a_1 \times 10^3$	$a_2 \times 10^5$	$a_3 \times 10^7$
1/3	−2.009	−1.617	1.421	−0.5562
1/5	−2.072	−0.5027	0.2110	−0.04031
1/7	−2.1022	−0.06649	−1.043	1.832
1/9	−2.120	−0.05078	−0.7230	1.827

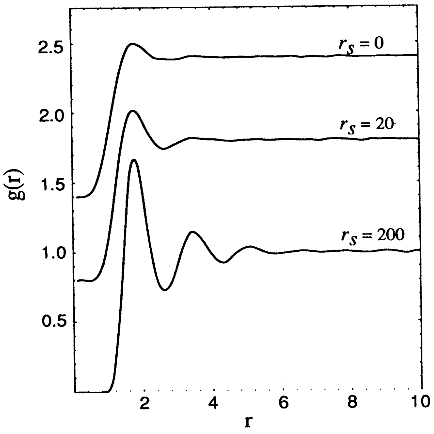

FIG. 2. Pair-correlation functions computed at $\nu = 1/3$ at various r_s.

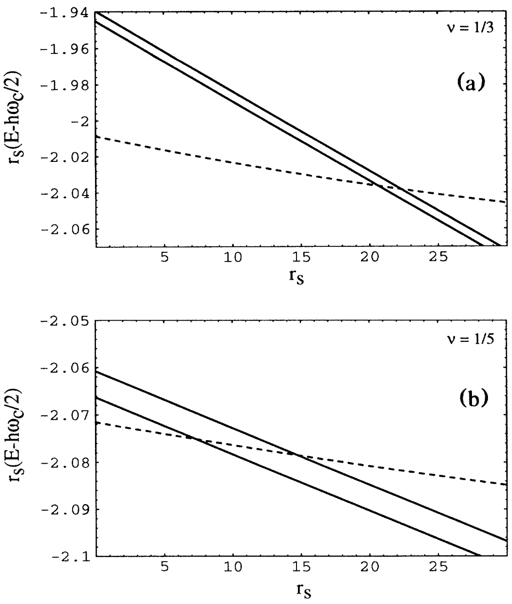

FIG. 3. Liquid and solid energies as a function of r_s for the $\nu = 1/3$ and $\nu = 1/5$ states. The dashed curves are liquid energies, and the solid lines are linear interpolations between the points at $r_s = 2$ and $r_s = 20$ of Zhu and Louie, both with and without impurities (assuming $\xi = 5a$).

the method given in [9], began with a harmonic Hamiltonian and computed the effect of the leading cubic term in second-order perturbation theory. For $\nu = 1/3$ he found that the cubic term lowered the energy of the harmonic solid by $-0.206\nu^2/r_s$ per particle, while the fourth-order term raised it by $0.290\nu^2/r_s$. The size of these energy shifts is, on the scale of the energy differences involved in the calculation, very significant. Higher-order terms are clearly required, but beyond fourth order the calculation becomes unmanageable, so as it stands these results are not useful.

Fortunately, however, a recent variational calculation of Zhu and Louie [10] which allows for Landau-level mixing gives us a nonperturbative upper bound for the solid energy. These authors modify the variational wave function of Lam and Girvin [8] by "squeezing" the Gaussian part of the wave function at each lattice site, such that

$$\exp(-\tfrac{1}{4}|z_i - R_i|^2) \rightarrow \exp(-\beta|z_i - R_i|^2), \tag{7}$$

and then multiplying by a Jastrow factor $e^{-\alpha/r^{1/2}}$. Varying α and β will vary the amount of Landau-level mixing in the wave function. Figures 3(a) and 3(b) are plots of the energy of the liquid (dashed line) and solid (solid lines) (Zhu and Louie) for $\nu = 1/3$ (a) and $\nu = 1/5$ (b) filling factors. This comparison implies that a phase transition to the solid will take place around $r_s \approx 22$ for $\nu = 1/3$ and at an $r_s \approx 15$ at $\nu = 1/5$.

In addition to all uncertainties connected with accuracy in the calculation for the liquid and solid energy in the absence of impurities, we must concern ourselves, at least qualitatively, with the effects of impurities. Even in the best samples we expect the electrons to couple to a rather slowly varying random potential produced by the dopant atoms, typically Si, offset from the interface by hundreds of angstroms. The electrons can in fact lower their energy somewhat by changing their local density to accommodate the local impurity potential. Since the liquid is incompressible at filling like $\nu = 1/3$, to lowest order in the potential fluctuations, it will not be able to do this. The solid, on the other hand, is compressible. For a weak smoothly varying potential, simple arguments based on an elastic medium description of the WS indicate that the energy gained by the solid is very roughly [16]

$$E_{\text{imp}} \approx \frac{1}{2} m v_t^2 \left(\frac{a}{\xi}\right)^2 = \frac{0.138}{r_s} \left(\frac{a}{\xi}\right)^2, \tag{8}$$

where $v_t = (0.138e^2/ma)^{1/2}$ is the transverse sound velocity in the absence of the magnetic field and ξ is the correlation length for the distorted WS. Depending on the quality of the sample, we might expect $5a < \xi < 50a$. If $\xi = 50a$, the effect on the solid energy will be minimal, and the solid energy will be given by the upper solid line in Fig. 3, whereas if $\xi = 5a$, the solid energy will be shifted to the value shown by the lower solid line. At $\nu = 1/3$ the solid energy crosses the liquid energy at a relatively large angle, so if we take $\xi = 5a$ the transition point may change by $\Delta r_s \approx 2$ or 3, but at $\nu = 1/5$, the slope of the two curves is more nearly equal, and the transition point may change by $\Delta r_s \approx 10$ or more. Of course, we do not know the coherence length, and Eq. (8) is only a rough estimate.

In Fig. 4 we have plotted the approximate phase boundary at zero temperature. The solid line with gaps in it is a phenomenological one-parameter Lindemann curve obtained by computing the mean-square relative

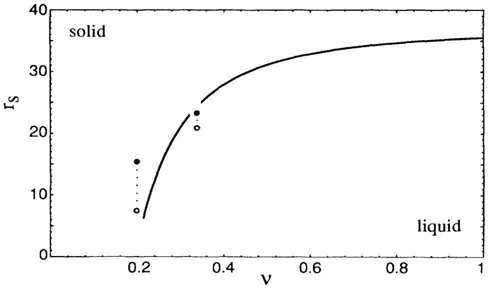

FIG. 4. The phase boundary between liquid and solid in terms of filling factor ν and density r_s. The solid curve is an estimate of the melting density from a phenomenological Lindemann criterion. The solid (open) dots are the phase transition points at $\nu = 1/3$ and $1/5$ computed assuming no ($\xi = 5a$) impurity shifts.

displacement of two atoms in a harmonic solid,

$$\Delta = \langle(\delta\mathbf{r}_i - \delta\mathbf{r}_{i+1})^2\rangle/a^2, \qquad (9)$$

and setting $\Delta = \Delta_c$. The value of Δ_c was chosen to agree with Ceperley's results [13] at $B = 0$. The gaps around the filling factors $\nu = 1/3$ and $1/5$ indicate that the curves must be quite rapidly varying. The solid dots are the values obtained from Fig. 3 in the absence of impurities, and the open dots are our worst-case estimate including impurities.

This variational calculation of the energy of the LL at finite density allows us to get a good semiquantitative picture of the phase boundary between WS and LL. Since high mobility hole doped samples in GaAs with $r_s \lesssim 15$ are now rather routinely available, this calculation suggests that there should be an interesting density dependence to much of the experimental data in the very best samples.

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