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LETTER TO THE EDITOR

Finite-size evidence for Wigner crystallization of 2D electrons in a magnetic field

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Abstract. Finite-size calculations are used to study the magnetic field dependence of the ground state of interacting 2D electrons. It is found that the pair correlation function acquires the hexagonal symmetry of a quantum Wigner crystal when the filling factor is between $\frac{1}{5}$ and $\frac{1}{7}$. The energy of the hexagonal state is compared with variational results for the Wigner crystal and the nature of the transition to hexagonal symmetry is briefly discussed.

Magnetic field induced Wigner crystallization of 2D electrons is currently under intense experimental study. In particular, techniques such as RF absorption [1], resistivity [2], threshold field studies [3] and threshold field studies combined with noise measurements [4] have recently been used to probe 2D electrons at GaAs–AlGaAs heterojunctions. The results indicate that the ground state is crystalline at filling factors less than $\frac{1}{5}$ and in a narrow range just greater than $\frac{1}{5}$ with a re-entrant liquid state very close to $\frac{1}{5}$ filling. Photoluminescence experiments also show anomalies at similar filling factors [5, 6, 7]. In addition there have been reports of re-entrant behaviour at odd denominator fillings less than $\frac{1}{5}$ [8]. There are also reports of Wigner crystallization in Si MOSFETS [9]. In comparison, the generally accepted theoretical picture is that the Wigner crystal state is energetically favourable when the filling factor is less than about $\frac{1}{6.5}$ [10]. However this estimate is based on comparison of variational energies so cannot be used to study the details of the transition. An alternative is to perform finite-size calculations [11] which has the advantage that the liquid and the crystal are treated in exactly the same way. This is the purpose the present work.

The results presented here come from exact diagonalization of the Hamiltonian for six electrons at filling factors down to $\frac{1}{9}$ and four electrons down to $\frac{1}{15}$. They represent a considerable advance on previous finite-size studies which have been restricted to filling factors down to around $\frac{1}{5}$. Nevertheless no radically new techniques were used to obtain them. Instead, the ability to probe very small fillings is the cumulative result of improvements in program efficiency and increased computer availability. Symmetry was used to reduce the size of the Hamiltonian as far as possible, including the use of rotational symmetry to give a twofold reduction in the size of the Hamiltonian in cases when translational symmetry gave little advantage. The ground state was found by standard iterative techniques (Lanczos or Davidson). In most cases it proved

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advantageous to use a starting vector made by prediagonalizing the Hamiltonian in a sub-space formed from a few of the lowest energy basis states since this reduced the number of iterations by a factor of about 2. However the prediagonalization sometimes failed at the smallest filling factors because it gave a vector near orthogonal to the ground state. In these cases a starting vector with equal components was used instead.

The calculations were done in the rectangular periodic geometry in a cell of height b and width a and the pair correlation function

$$g(r) = \frac{ab}{n(n-1)}\left\langle \sum_{i\neq j} \delta(r - r_i + r_j) \right\rangle$$

was used to look for signs of crystalline order. Here the angled brackets denote the ground state expectation value and n is the number of electrons. Of course it is impossible to study *long range* order in a finite-size calculation, but it is possible to determine whether there is any short range order which is consistent with a Wigner crystal of a particular symmetry. Since the classical Wigner crystal of lowest energy is hexagonal [12] the aspect ratio $R = b/a$ of the rectangular cell was chosen to be compatible with hexagonal symmetry (i.e. $R = 1/\sqrt{3}$ when for $n = 6$ and $R = \sqrt{3}/2$ for $n = 4$). The use of rectangular periodic boundary conditions means that the hexagonal symmetry is not imposed on the system but the special choice of aspect ratio does not exclude it. The emergence of this symmetry is therefore taken to be the signature of Wigner crystallization although it is also consistent with a hexatic phase which is predicted to occur at higher temperatures than the crystal [13].

Results for the ground state pair correlation function at filling factors of $\frac{1}{3}$, $\frac{1}{6}$ and $\frac{1}{9}$ are shown in figure 1. It is clear that the ground state evolves from one which is liquid-like at $\nu = \frac{1}{3}$ to one which has hexagonal symmetry $\nu = \frac{1}{9}$. Further evidence for a crystalline state at $\nu = \frac{1}{9}$ comes from the structure factor and the symmetry of the excited state dispersion relation. In the limit of infinite magnetic field the components of the cyclotron orbit centre operators commute [14] and the orbit centres should form a lattice. Hence it is natural to examine the cyclotron orbit centre structure factor, $S_o(q)$ which is related to the usual $S(q)$ by

$$S(q) = 1 - \exp(-q^2l^2/2) + \exp(-q^2l^2/2)S_o(q)$$

where $l^2 = \hbar/eB$ is the square of the magnetic length [15]. This quantity is shown in figure 2. The lower right frame illustrates the correspondence between the rectangular reciprocal space of the finite-size calculation and the hexagonal reciprocal space of the Wigner crystal. The rectangular grid indicates the reciprocal space points accessible in the six-electron finite-size calculation at 1/integer filling and the bold lines show the reciprocal lattice of the hexagonal crystal. The rectangle $\Gamma JKJ'$ is the irreducible rectangle in the Brillouin zone of the rectangular cell while the dotted line shows part of the Brillouin zone of the hexagonal lattice; the points X_h and J_h are the high symmetry points of this zone. The four left hand frames show $S_o(q)$ along the Wigner crystal reciprocal lattice directions (Γ J and (3,1)) at $\nu = \frac{1}{3}$ and $\nu = \frac{1}{9}$. The length of q is measured by the number of points in the indicated direction, starting from Γ, and the arrows indicate the reciprocal lattice points of the Wigner crystal. It is clear that at $\nu = \frac{1}{3}$ $S_o(q)$ has almost no peaks at the reciprocal lattice vectors of the Wigner crystal but the largest peaks occur at these vectors at $\nu = \frac{1}{9}$. Similar

behaviour is found when $S_0(q)$ is examined along the $\Gamma J'$ direction. As the ground state acquires hexagonal symmetry its excitation spectrum also acquires hexagonal symmetry and this can be verified by looking at the energy dispersion $E(k)$. (The assignment of k-values is as described by Maksym [16].) Since the hexagonal lattice has higher symmetry than the rectangular lattice some of the eigenvalues become near degenerate at the onset of hexagonal symmetry and this is consistent with softening of the roton mode of the liquid ground state [17]. For example, in figure 2 the points Γ, (0,2), K and (3,1) would be equivalent if the hexagonal symmetry was exact. Similar considerations show that the 16 k-points in the irreducible rectangle $\Gamma JKJ'$ become equivalent to four sets of four points as the system becomes hexagonal. Consequently the eigenvalues merge into four near-degenerate multiplets. The onset of this behaviour is shown in the bottom right frame of figure 2. This gives the lowest eigenvalue at each k-point in the rectangular Brillouin zone at $\nu = \frac{1}{3}$ and $\nu = \frac{1}{9}$. The energies are per electron, measured in units of $(e^2/4\pi\epsilon\epsilon_0)\sqrt{2\pi/ab}$. The lowest four eigenvalues at $\nu = \frac{1}{9}$ are near degenerate and occur at the k-points expected from symmetry considerations as are three of the eigenvalues belonging to the highest multiplet. The fourth lies between eigenvalues of the two intermediate multiplets and there is further interweaving of the eigenvalues belonging to these multiplets. Calculations for four electrons have shown that the interweaving persists until the filling factor is $\frac{1}{15}$ when all the eigenvalues lie in near-degenerate multiplets, as expected for hexagonal symmetry.

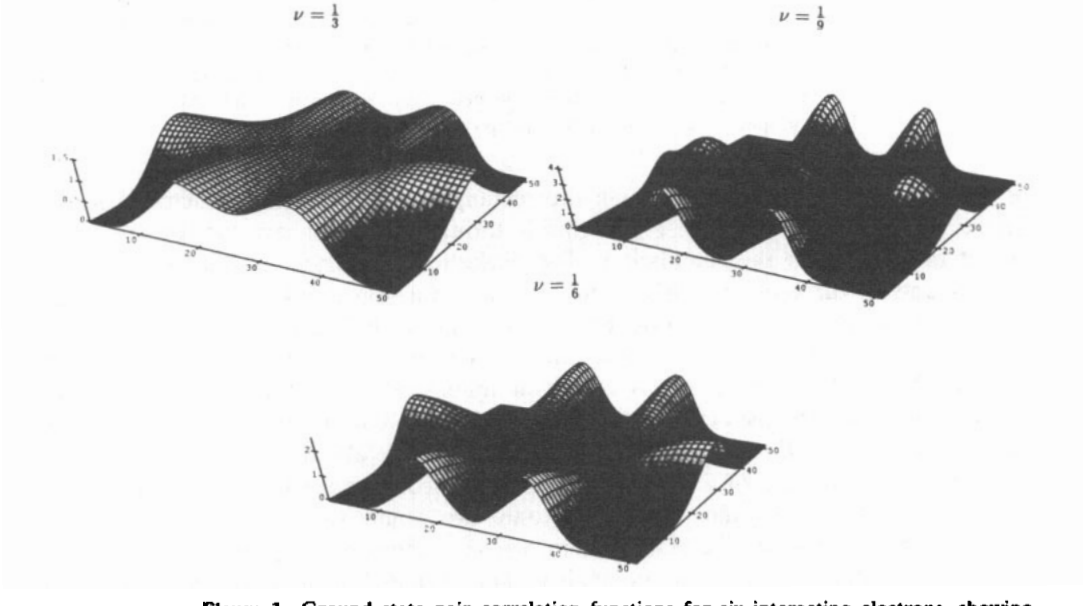

Figure 1. Ground state pair correlation functions for six interacting electrons, showing the emergence of hexagonal symmetry with decreasing filling.

The ground state energy as a function of magnetic field is also consistent with the disappearance of the liquid ground states. One signature of the liquid ground state is a cusp-like minimum in the ground state energy as a function of magnetic field as can be seen at $\nu = \frac{1}{3}$ and $\nu = \frac{1}{5}$ in figure 3. This shows the ground state energy per electron in units as in figure 2 against magnetic field in units of the number

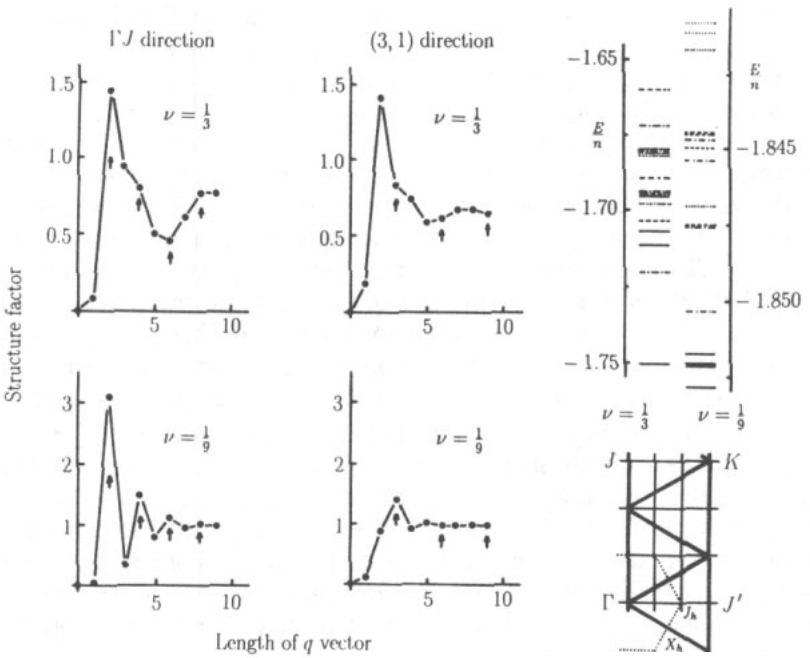

Figure 2. Comparison of structure factors and excitation spectrum for six electrons at $\nu = \frac{1}{3}$ and $\nu = \frac{1}{9}$. Structure factors are shown in the four left hand frames. The bottom right frame illustrates the corresponding reciprocal space and the top right frame shows the excitation spectrum. Different line styles indicate eigenvalues that belong to near degenerate multiplets in the large field limit: solid line: Γ multiplet; dotted line: (1,0) multiplet; broken line: (2,0) multiplet; chained line: (3,0) multiplet.

of magnetic flux quanta, m, through the rectangular cell; the filling factor is n/m. There is also a cusp at $\nu = \frac{1}{2}$ but this is thought to be an artefact of the small aspect ratio used for the calculation. The periodic boundary conditions force the x components of the cyclotron orbit centres to lie on a grid of spacing $\Delta X = 2\pi l^2/b$ and in a real system the magnetic length is always much larger that the orbit centre spacing i.e. $l \gg \Delta X$. Together with the relation $m = ab/2\pi l^2$, this requirement leads to the condition $m \gg 2\pi/R$ and even denominator minima occur in finite-size calculations when the aspect ratio is so small that this condition is not satisfied [18]. For six electrons at $R = 1/\sqrt{3}$ the critical value of m is about 11 which is very close to $\nu = \frac{1}{2}$. The absence of a minimum at $\nu = \frac{1}{7}$ is consistent with the disappearance of the liquid state. Beyond 6/43 filling only two points ($\nu = \frac{1}{8}$ and $\nu = \frac{1}{9}$) are shown in the figure since the Hamiltonian matrix at the remaining points is too big to handle. The energy at these two points is within 0.5% of Lam and Girvin's variational calculation of the Wigner crystal ground state energy [10]. It is also within 0.3% of a calculation due Meissner and Brockstieger [19] but for clarity only the Lam–Girvin result is shown. At $\nu = \frac{1}{9}$ the exact ground state energy is about 3% higher than the energy of a classical Wigner Bravais lattice [12] (broken line) but the difference drops to about 2% at $\nu = \frac{1}{15}$.

The behaviour of the four-electron system in the near-classical regime at $\nu = \frac{1}{15}$ was investigated quantitatively by examining its shear modulus and its excitations. The shear modulus was obtained from the difference between the energy of the

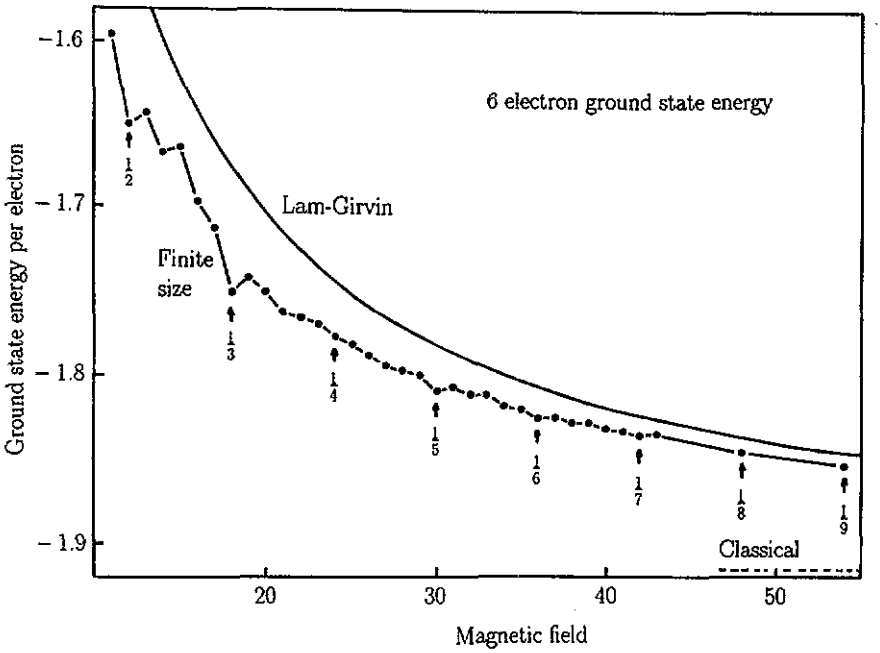

Figure 3. Ground state energy per electron against magnetic field. The points give the six electron ground state energy and the lines joining them are to guide the eye. Units are given in the text.

system in a rectangular periodic cell and the energy in an oblique cell of the same height. This gives a shear modulus of $0.20(n/ab)^{3/2}$ compared with the classical value of $0.245(n/ab)^{3/2}$ [12]. Because the eigenvalues at $\nu = \frac{1}{15}$ lie in near-degenerate multiplets, the excitation energies of the four-electron system are available at only two k-points of the hexagonal Brillouin zone, namely X_h and $3/4$ along ΓJ_h. The corresponding frequencies are $3\omega_o \pm 20\%$ and $4.6\omega_o \pm 20\%$ where the error comes from the spread of eigenvalues within each near-degenerate multiplet. The frequency ω_o is defined by $\omega_o = \Omega^2/\omega_c$ where $\Omega = e^2/(4\pi\epsilon\epsilon_0 m^* \alpha^3)$, $\alpha^2 = (2ab)/(n\sqrt{3})$ and ω_c is the cyclotron frequency. These frequencies can be compared with results for the classical Wigner crystal given by Meissner and Brockstieger [19] which, when extrapolated to $\nu = \frac{1}{15}$, are $4.2\omega_o$ and $5.7\omega_o$ respectively. Thus the classical frequencies lie above the exact ones which is consistent with the lower shear modulus of the finite-size system. The extent to which this is a finite-size effect is not yet clear.

Since the finite-size calculation treats the liquid and the crystal in the same way it allows the evolution of the crystal state to be followed directly. It is found that the three peaks in $g(r)$ along the line $y = 0.5b$ develop slowly as the filling factor decreases from $\nu = \frac{1}{5}$ to $\nu = \frac{1}{7}$. Around $\nu = \frac{1}{5}$ there are only two peaks on the line $y = 0.5b$. Their positions are $(0, 0.5b)$ and $(a, 0.5b)$ and they are equivalent because of the periodic boundary conditions. The central peak (at $(0.5a, 0.5b)$) is absent at this filling. With decreasing ν the two side peaks sharpen and move inwards, while the central one gradually develops. When the filling factor is just below $\frac{1}{7}$ all three peaks are within 2% of the positions expected for a hexagonal lattice. This is consistent with Lam and Girvin's theoretical result for the filling factor at which the

Wigner crystal becomes energetically favourable but inconsistent with experimental observation of crystal states at fillings just greater than $\frac{1}{5}$. The behaviour close to $\nu = \frac{1}{7}$ is much more interesting and is shown in figure 4. This shows the ground state pair correlation functions at exactly $\nu = \frac{1}{7}$ and one flux quantum away from this filling, i.e. at $\nu = \frac{6}{41}$ and $\nu = \frac{6}{43}$. While the ground states on either side of $\nu = \frac{1}{7}$ are clearly hexagonal the hexagonal features at exactly $\nu = \frac{1}{7}$ are washed out although there are excited states which do have hexagonal symmetry. (The loss of hexagonal symmetry is most clearly evident along the line $y = 0.5b$.) This suggests a tendency for the liquid state to reform at $\nu = \frac{1}{7}$ and is possibly consistent with the re-entrant behaviour reported by Buhmann *et al* [8]. However this conclusion must remain tentative as it is impossible to rule out other explanations such as finite-size effects.

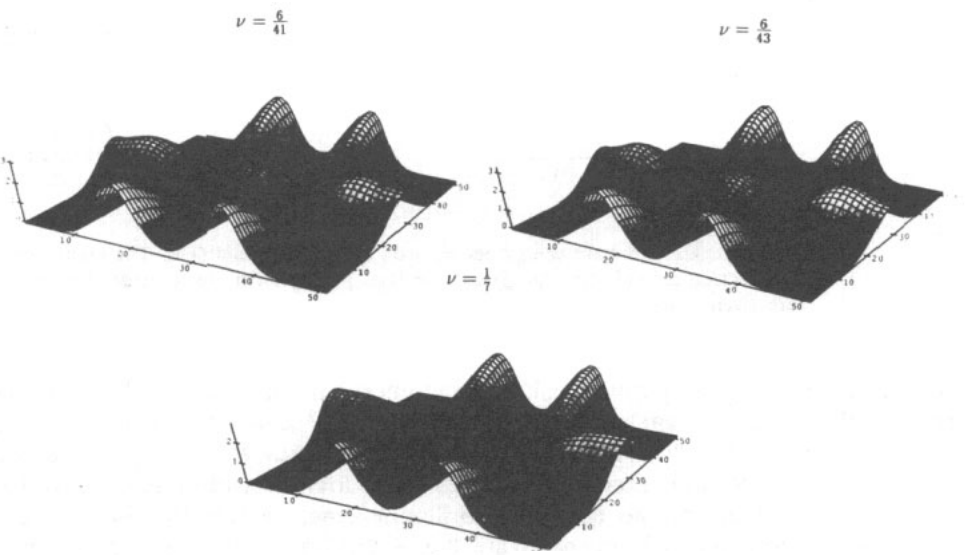

Figure 4. Ground state pair correlation functions for $\nu = \frac{1}{7}$ and one flux quantum to each side of $\nu = \frac{1}{7}$, showing disappearance of hexagonal symmetry at exactly $\nu = \frac{1}{7}$.

In summary, finite-size calculations have been used to study Wigner crystallization of 2D electrons. A state of hexagonal symmetry evolves from the liquid state when the filling factor is in the range between $\frac{1}{5}$ and $\frac{1}{7}$ and its energy is close to variational estimates of the Wigner crystal energy. Around $\frac{1}{15}$ filling the crystal appears to be near-classical. There are indications of interesting behaviour when the filling factor passes through exactly $\frac{1}{7}$.

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