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2004 J. Phys.: Condens. Matter 16 L271

(http://iopscience.iop.org/0953-8984/16/21/L01)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **16** (2004) L271–L277 PII: S0953-8984(04)79854-9

LETTER TO THE EDITOR

Composite-fermion crystallites in quantum dots

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Received 27 April 2004
Published 14 May 2004
Online at stacks.iop.org/JPhysCM/16/L271
DOI: 10.1088/0953-8984/16/21/L01

Abstract

The correlations in the ground state of interacting electrons in a two-dimensional quantum dot in a high magnetic field are known to undergo a qualitative change from liquid-like to crystal-like as the total angular momentum becomes large. We show that the composite-fermion theory provides an excellent account of the states in both regimes. The quantum mechanical formation of composite fermions with a large number of attached vortices automatically generates composite fermion crystallites in finite quantum dots.

(Some figures in this article are in colour only in the electronic version)

The system of interacting electrons confined to a two-dimensional quantum dot and exposed to a strong magnetic field has been a subject of intense theoretical study for over two decades [1–14], both because such quantum dots have been realized and studied in the laboratory [15–17], and because of the possible relevance of their physics to the fractional quantum Hall effect (FQHE) [18]. For systems with small numbers of particles, exact diagonalization can be performed for parabolic quantum dots in the limit when the cyclotron energy is large compared to the confinement potential, which shows that the ground state energy as a function of the angular momentum (L) has a rather rich structure. In particular, downward cusps appear at certain values of L, which are consequently especially favourable. An understanding of the correlations in the quantum dot state that underlie this physics is one of the central questions for this system. One would also like to know how this ties into our understanding of the FQHE, obtained in the thermodynamic limit without confinement.

The approach based on the formation of composite fermions has been demonstrated to be successful in a range of L values [8, 9]. Specifically, a mean-field type description, in which the composite fermions are taken as non-interacting particles at an effective angular momentum L^*, with their mass or the cyclotron energy treated as a phenomenological parameter, predicts cusps in the energy at certain magic angular momenta, which are in agreement with the actual cusp positions in exact diagonalization studies [8]. However, discrepancies appear at large L [10, 12]; here, the actual cusps occur at regular intervals in L, which has been interpreted

in terms of classical crystal-like states [13]. At large L, the repulsive interaction thus appears to stabilize a (rotating) crystal rather than a liquid, which is believed to signal a breakdown of the composite-fermion (CF) description. That would not be unexpected, because large angular momenta correspond to small filling factors (to the extent that the filling factor is a meaningful quantity in a finite quantum dot), and it is known, for infinite two-dimensional systems, that the CF liquid gives way to a Wigner crystal at sufficiently small fillings.

To understand the nature of the breakdown of the composite fermion description, a matter of great interest also in the context of the FQHE, we have undertaken an extensive study of finite systems at large angular momenta. Our investigations, however, have led to a surprising conclusion: even though the naive *mean-field* interpretation in terms of *free* composite fermions becomes invalid at large L, the microscopic composite fermion theory, defined through wavefunctions, continues to give a very good description down to the largest L studied to date. It provides an accurate approximation for the ground state wavefunction and the ground state energy at every single L in the wide range studied, and correctly reproduces all cusps in a plot of the ground state energy versus L. Taken together, these results constitute a detailed verification for the validity of the composite fermion theory for quantum dots even at very low fillings.

This may appear to be at odds with the classical crystal-like correlations found in exact diagonalization studies [10, 14]. While both composite fermions and the crystal are generated by the repulsive interaction between electrons, the feeling has been that one excludes the other. A notable aspect of our work is the unexpected finding that not only is there no logical inconsistency between the simultaneous formations of composite fermions and crystal-like structures at low fillings, but that the state is very well described as a crystallite of composite fermions.

The Hamiltonian of interest is

$$H = \sum_j \frac{1}{2m_\mathrm{b}} \left(\boldsymbol{p}_j + \frac{e}{c}\boldsymbol{A}_j \right)^2 + \sum_j \frac{m_\mathrm{b}}{2}\omega_0^2 r_j^2 + \sum_{j<k} \frac{e^2}{\epsilon r_{jk}}, \tag{1}$$

where m_b is the band mass of the electron, ω_0 is a measure of the strength of the confinement, ϵ is the dielectric constant of the host semiconductor, and $r_{jk} = |\boldsymbol{r}_j - \boldsymbol{r}_k|$. We will specialize to the case of very large magnetic fields, when $\omega_c = eB/m_\mathrm{b}c \gg \omega_0$. Only the lowest Landau level (LL) is relevant in this limit. In that limit, at each angular momentum the eigenenergy neatly separates into a confinement part and an interaction part:

$$E(L) = E_c(L) + V(L), \tag{2}$$

where $E_c(L) = (\hbar/2)[\Omega - \omega_c]L$, relative to the lowest LL, with $\Omega^2 = \omega_c^2 + 4\omega_0^2$, and $V(L)$ is the interaction energy of electrons without confinement, but with the magnetic length replaced by an effective magnetic length given by $\ell \equiv \sqrt{\hbar/m_\mathrm{b}\Omega}$. In the following, we will only consider V as a function of the angular momentum L; it must be remembered, however, that the confinement part must eventually be added to determine the global ground state. The exact ground state in each L sector is obtained by either matrix diagonalization or the Lanczos method. The largest system we have studied has a Fock space dimension of 509 267.

In the CF theory [3, 8, 19], the interacting state of electrons in the lowest LL at angular momentum L is mapped into the non-interacting electron state at L^*, where

$$L = L^* + pN(N-1), \tag{3}$$

N is the number of electrons, and p is an integer. The wavefunctions are related as

$$\Psi_\alpha^L = \mathcal{P} \prod_{j<k} (z_j - z_k)^{2p} \Phi_\alpha^{L^*}. \tag{4}$$

Here $\Phi_\alpha^{L^*}$ are the wavefunctions for non-interacting electrons at L^* (which in general occupy several Landau levels), $\alpha = 1, 2, \ldots, D^*$ labels the different states, $z_j = x_j - \mathrm{i}y_j$ denotes the position of the jth electron, $\mathcal{P}$ indicates projection into the lowest LL, Ψ_α are basis functions for interacting electrons at L, and D^* is the dimension of the CF basis. We will restrict Φ_α to states with the lowest kinetic energy at L^*, and choose p so as to have the smallest dimension for the basis. The composite fermions carrying $2p$ vortices are labelled ^{2p}CFs. At certain values of L, the above prescription produces only one state ($D^* = 1$), which is the CF theory's answer for the ground state. In the notation of [8], this is a compact state, denoted by $(N_0, N_1, \ldots)$, with N_j composite fermions compactly occupying the innermost angular momentum orbitals of the jth CF level. At other values of L, when there are many CF basis states ($D^* > 1$), we diagonalize the Coulomb Hamiltonian in the CF basis to obtain the ground state, using methods described earlier [9, 20]. For any N, there are many values of L where the CF theory gives a unique answer, but in general, D^* increases with N.

We have carried out exact diagonalization for $N \leqslant 8$. It is possible to go to arbitrarily large values of L within the CF theory, but available computer memory has restricted our *exact* diagonalization study to $L \leqslant 135, 117$ and 111 for $N = 6$, 7 and 8, respectively. Figure 1 shows the comparison between the CF theory and the exact energy as a function of L for $N = 6$ particles, demonstrating that the CF theory predicts every energy accurately and obtains all cusps faithfully[1]. The comparisons for other values of N are similar.

We next come to the connection between our approach and the crystalline correlations found in previous studies. Such correlations are not manifest in the density, which is rotationally symmetric for the ground state with a definite angular momentum, so one must compute the pair correlation function

$$g(\boldsymbol{r}) \sim \int \prod_{j=3}^{N} \mathrm{d}^2\boldsymbol{r}_j |\Psi(\boldsymbol{r}, \boldsymbol{R}, \boldsymbol{r}_3, \ldots, \boldsymbol{r}_N)|^2, \tag{5}$$

which is the probability of finding a particle at $\boldsymbol{r}$ while holding one particle fixed at $\boldsymbol{R}$. We first compute the density as a function of the distance from the centre, and fix $\boldsymbol{R}$ somewhere on the maximum density ring. As an example, figure 2 (upper panel) shows the exact pair correlation function for six particles at $L = 95$, which clearly illustrates crystallite formation. The CF theory gives a unique state here, (4, 2), which has the wavefunction (with $N = 6$ and $2p = 6$)

$$\Psi = \mathcal{P}A\left[z_1^* z_2 z_2^* \prod_{i=3}^{N} z_i^{i-3}\right] \prod_{j<k} (z_j - z_k)^{2p} \mathrm{e}^{-\sum_{l=1}^{N} |z_l|^2/4}, \tag{6}$$

where A denotes an antisymmetric Slater determinant. The projection is accomplished by the method outlined in the literature [9]. The energy of this wavefunction is $1.955\,35(15)e^2/\epsilon\ell$, which compares well with the exact energy $1.950\,61e^2/\epsilon\ell$. The overlap with the exact ground state is 0.902. The pair correlation function for this wavefunction is also shown in figure 2 (lower plot). It is remarkable that the single wavefunction from the CF theory provides a good qualitative and quantitative description of the actual ground state wavefunction in figure 2, which is a linear combination of 69 624 basis functions. We have studied other 'cusp states' and found similarly good agreement.

The composite fermion wavefunction at any angular momentum L is obtained from *non*-interacting electron wavefunction at an effective angular momentum L^* by multiplication

[1] It so happens for $N = 6$ that for one point in each panel of figure 1, the smallest dimension D^* is obtained with an anomalous value of $2p$. We actually get a slightly better CF energy if we instead choose here $2p$ that matches $2p$ for other L in the panel.

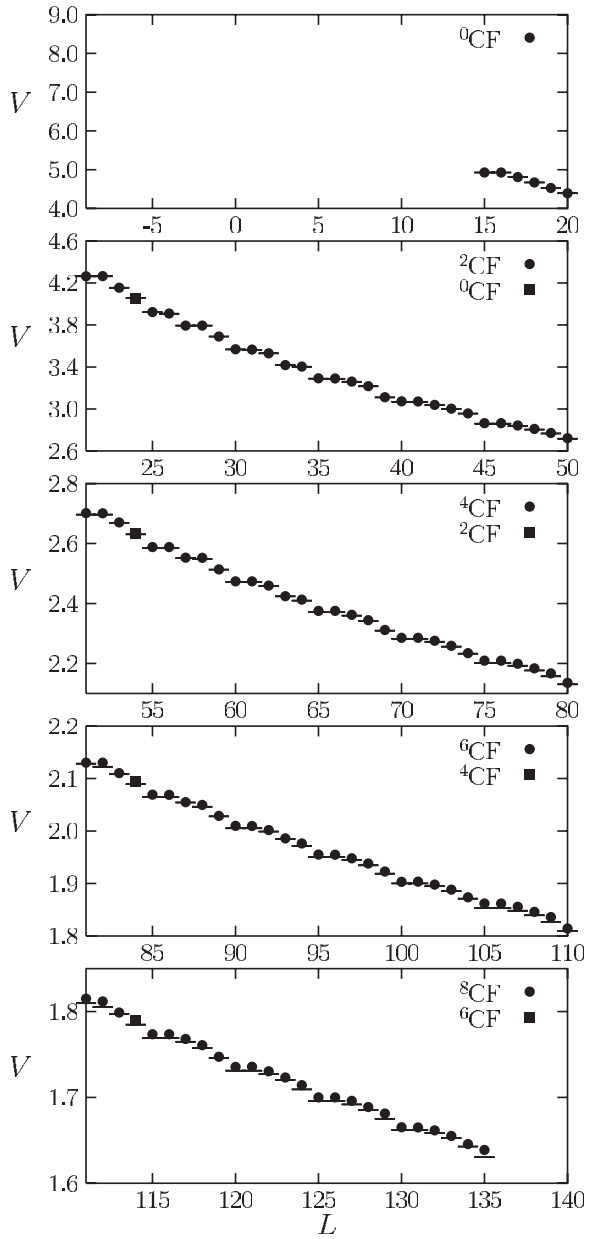

Figure 1. The exact interaction energy V (dashes) is given as a function of the angular momentum L for $N = 6$ particles. The dots are the predictions of the CF theory. Different panels correspond to L regions where composite fermions of different flavours are relevant. (In each panel, for L related to $L^* = -6$, the lower order CF gives a smaller D^*.) The energies are quoted in units of $e^2/\epsilon\ell$.

by an appropriate Jastrow factor, in exactly the same way as wavefunctions are written for bulk fractional quantum Hall states. It is crucial to note that no physics of any kind of crystal is put into these wavefunctions by hand at any stage. For example, referring to figure 2, the parent electron wavefunction at $L^* = 5$, namely $A[\cdots]$ in equation (6), has

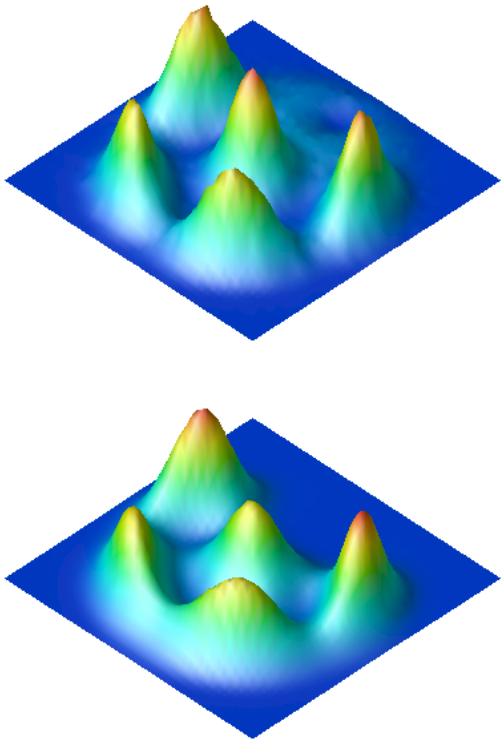

Figure 2. The upper plot shows the pair correlation functions for the exact ground state for $N = 6$ particles at $L = 95$, and the lower plot displays the prediction of the CF theory. The exact ground state is a linear superposition of 69 624 basis states, whereas the ^{6}CF ground state is given by a unique wavefunction denoted by (4, 2). The 'missing peak' on the outer ring indicates the location $\boldsymbol{R}$ of the fixed particle.

no crystalline correlations in it. It describes a simple *non-interacting* system with single particle orbitals $\{0, 0\}$, $\{0, 1\}$, $\{0, 2\}$, $\{0, 3\}$, $\{1, -1\}$, and $\{1, 0\}$ occupied, where $\{n, m\}$ denotes the angular momentum m orbital in the nth LL. (The allowed values are $n = 0, 1, \ldots$, and $m = -n, -n + 1, \ldots$.) However, when the uncorrelated wavefunction at L^* is multiplied by an appropriate Jastrow factor to convert electrons into composite fermions, the resulting wavefunction describes a correlated electron liquid for a certain range of L values, but for sufficiently large angular momenta it produces a state with crystalline correlation; in other words, the formation of composite fermions automatically causes the formation of a crystallite at large L. It is stressed that the same class of wavefunctions describes both the liquid and the crystal in quantum dots in different parameter regimes. The emergence of such classical crystal-like structures in the intrinsically quantum mechanical state of composite fermions is striking.

To investigate the evolution with the number of attached vortices, we show in figure 3 the pair correlation function for $N = 19$ composite fermions in the state (17, 2) (with wavefunction given in equation (6)) for three flavours of composite fermions, with $2p = 2$, 10, and 20. The crystal becomes better defined with increasing $2p$. In this case, we do not have exact results to compare with (the dimension of the Fock space is astronomically large; even for the smallest system in figure 3, namely 19 particles at $L = 477$, it is estimated to be 10^{14}), but the structure at large L is consistent with classical considerations that predict a three-ring

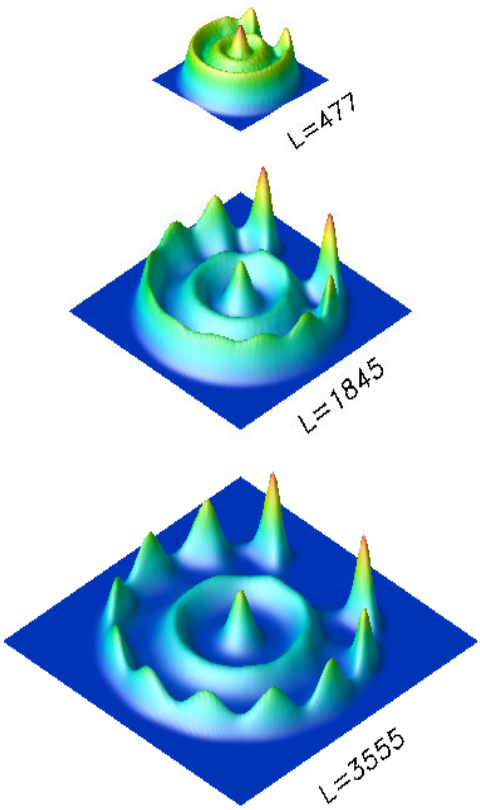

Figure 3. Pair correlation functions for the (17, 2) configuration for $N = 19$ composite fermions of three different flavours, namely ^{2}CFs, ^{10}CFs, and ^{20}CFs (from top to bottom). The missing peak on the outer ring indicates the location $\boldsymbol{R}$ of the fixed particle. The three figures are plotted on the same length scale to illustrate how the size grows with L.

structure with 1, 6 and 12 electrons located on inner, middle and outer rings, respectively [21]. Interestingly, when we hold a particle in the middle ring fixed, the hexagonal correlations of the middle ring become prominent while the outer ring becomes more or less uniform. That is consistent with earlier studies that show that the radial correlations between different rings are weaker than the angular correlations within a ring, producing, for example, two different melting transitions [22].

A recent article by Yannouleas and Landman [12] has asserted that the CF theory fails to produce the cusp positions for large L, especially beyond $L > 75$ (for $N = 6$). That assertion is not borne out by our results, which demonstrate that the CF theory, when taken beyond the most naive mean field picture, predicts each cusp correctly at least for angular momenta up to $L = 135$. Yannouleas and Landman [12] have studied an alternative trial wavefunction based on an analogy to the classical crystal ground state in a quantum dot. A thorough comparison of the CF theory and the approach of [12] is not possible because the latter obtains wavefunctions and energies only for certain special values of L. For $N = 6$, [12] explicitly quotes energies from their approach for seven values of L in the range $75 \leqslant L \leqslant 135$. For these seven angular momenta, the CF theory gives lower energy in every case except at $L = 135$. In future, it would be interesting to compare the two methods for a larger range of L and N to ascertain their respective regimes of validity.

One may ask what implications our results have for the nature of the bulk FQHE state at small fillings. While the finiteness of the systems does not allow us to draw a firm conclusion regarding whether the thermodynamic state at some filling is a liquid or a crystal, the results do indicate that the CF state possesses a substantial short-range crystalline order at small ν. This raises the interesting issue of whether the actual Wigner crystal at low fillings is a crystal of electrons or of composite fermions [23].

The composite fermion description of correlated electron states in quantum dots at high magnetic fields has several appealing features: it gives a unified theory, applicable to angular momenta spanning *both* the liquid and the crystal phases; it produces microscopic wavefunctions also for those angular momenta where no classically stable crystal is available; it obtains the correct crystal shape and the ring structure without an explicit consideration of the classical solution; and finally, through CF theory, the understanding of the quantum dot physics dovetails nicely with that of the FQHE. Before ending, we note that the accuracy of the CF wavefunctions can be improved straightforwardly and systematically by enlarging the basis at L^* slightly [24]; the goal in this work was to demonstrate that the zeroth order theory itself works very well.

Partial support by the National Science Foundation under grant no. DMR-0240458 is gratefully acknowledged.

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