Semiconductor quantum dots in high magnetic fields: The composite-fermion view

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We review and extend the composite fermion theory for semiconductor quantum dots in high magnetic fields. The mean-field model of composite fermions is unsatisfactory for the qualitative physics at high angular momenta. Extensive numerical calculations demonstrate that the microscopic CF theory, which incorporates interactions between composite fermions, provides an excellent qualitative and quantitative account of the quantum dot ground state down to the largest angular momenta studied, and allows systematic improvements by inclusion of mixing between composite fermion Landau levels (called A levels).

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I. INTRODUCTION

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.1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25 Such quantum dots have been observed and studied in the laboratory.26,27,28,29 Exact diagonalization studies show that the ground states are strongly correlated, and the aim of theory is to achieve a satisfactory understanding of the correlations. It is also of interest to understand how this ties into our understanding of the FQHE,30 obtained in the thermodynamic limit without confinement.

The CF theory has been applied to parabolic quantum dots subjected to a strong magnetic field. The plot of ground state energy as a function of the angular momentum (L) has a rich structure. In particular, the ground state energies are strongly correlated, and the aim of theory is to achieve a satisfactory understanding of the correlations. It is also of interest to understand how this ties into our understanding of the FQHE,30 obtained in the thermodynamic limit without confinement.

The work in Ref. 32 showed that no logical inconsistency exists between the simultaneous formations of composite fermions and crystal-like structures at low fillings, and, furthermore, the formation of composite fermions itself induces crystal structure at low fillings. This crystal has been shown to be very well described as a crystal of composite fermions.33,34

The aim of this paper is to review and extend the CF theory of quantum dots in high magnetic fields, and also provide many details left out in earlier papers. Section II briefly outlines the basics of the CF theory for quantum dot states, giving explicit wave functions for some simple cases. Section III describes the numerical methods (exact diagonalization, Lanczos, and CF diagonalization). The mean-field CF model is discussed in Sec. IV, and the “zeroth-order” CF diagonalization in Sec. V. Section VI illustrates how the results are improved by going to higher orders in the CF theory. The paper is concluded in Sec. VII.

II. THE COMPOSITE-FERMIOM BASICS FOR QUANTUM DOTS

Following the standard practice, we assume below parabolic confinement. This should be a good approximation for most quantum dots at low energies, and simplifies calculations because of the availability of exact solutions for single particle eigenstates. The Hamiltonian of interest is

\[ H = \sum_j \frac{1}{2m_b} \left( p_j + \frac{e}{c} A_j \right)^2 + \sum_j \frac{m_b}{2} \omega_0 r_j^2 + \sum_{j<k} \frac{e^2}{r_{jk}}, \]

where \( m_b \) is the band mass of the electron, \( \omega_0 \) is a measure of the strength of the confinement, \( e \) is the dielectric constant of the host semiconductor, and \( r_{jk} \equiv |r_j - r_k| \). We will specialize to the case of very large magnetic fields, when \( \omega_c \equiv eB/m_b c \gg \omega_0 \). Only the lowest Landau level (LL) is relevant in this limit. In that limit, at each angular momentum the eigenenergy neatly separates into a
be added to determine the global ground state.

It must be remembered, however, that the confinement part must be added to determine the global ground state. In the CF theory, the interacting state of electrons in the lowest LL at angular momentum \( L \) is mapped into the noninteracting electron state at \( L^\ast \), where

\[
L = L^\ast + pN(N-1),
\]

where \( p \) is an integer. The wave functions

\[
\Psi^L = \mathcal{P}_{LLL} \prod_{j<k} (z_j - z_k)^{2p} \Phi^{L^\ast}
\]

give ansatz wave functions for interacting electrons at \( L \) in terms of the known wave functions of noninteracting electrons at \( L^\ast \). Here \( \Phi^{L^\ast} \) are the wave functions for noninteracting electrons at \( L^\ast \) (which in general occupy several Landau levels), \( \alpha = 1, 2, \cdots, D^\ast \) labels the different states, \( z_j = x_j - iy_j \) denotes the position of the \( j \)-th electron, \( \mathcal{P}_{LLL} \) indicates projection into the lowest LL, \( \Psi^L \) are basis functions for interacting electrons at \( L \), and \( D^\ast \) is the dimension of the CF basis. We will restrict \( \Phi^{L^\ast} \) to states with the lowest kinetic energy at \( L^\ast \), and choose \( p \) so as to have the smallest dimension for the basis. The composite fermions carrying \( 2p \) vortices are labeled \( \text{CF}^p \)'s. At certain values of \( L \), the above prescription produces only one state (\( D^\ast = 1 \)), which is the CF theory's answer for the ground state. In the notation of Ref. \( 10 \), this is a compact state, denoted by \([N_0, N_1, \cdots] \), with \( N_j \) composite fermions compactly occupying the innermost angular momentum orbitals of the \( j \)-th CF level. At other values of \( L \), when there are many CF basis states (\( D^\ast > 1 \)), we diagonalize the Coulomb Hamiltonian in the CF basis to obtain the ground state, using methods described earlier. For any \( N \), there are many values of \( L \) where the CF theory gives a unique answer, but in general, \( D^\ast \) increases with \( N \).

A. \( \text{Examples of CF bases} \)

Construction of the CF basis is in principle straightforward. We consider some explicit examples. In many cases, the CF basis consists of a unique wave function, which simplifies the analysis tremendously. The simplest wave function is the one for one filled \( \Lambda \) level (CF Landau level), shown schematically in Fig. 1(a):

\[
\Psi = A \prod_{k=1}^{N} \frac{z_i^{(4)}}{z_i^{(2)}} \Phi^{2p} = \prod_{j<k} (z_j - z_k)^{2p+1} e^{-\sum_{k=1}^{N} |z_i|^2/4},
\]

where \( A \) denotes an antisymmetric Slater determinant, i.e.

\[
A \left[ \prod_{i=1}^{N} z_i^{-1} \right] = \begin{vmatrix}
1 & 1 & \cdots & 1 \\
z_1 & z_2 & \cdots & z_N \\
\vdots & \vdots & \ddots & \vdots \\
z_{N-1} & z_{N-1} & \cdots & z_N^{-1} \\
\end{vmatrix} = \prod_{j<k} (z_j - z_k)
\]
FIG. 2: Schematic depiction of basis states at (a) \( L = 33 \); (b) \( L = 34 \) for \( N = 6 \) particles.

It corresponds to \( L = (2p + 1)N(N - 1)/2 \). It is identical to the Laughlin wave function.

The state \([N - 1, 1]\) at \( L = (2p + 1)N(N - 1)/2 - N \), shown in Fig. 2(b), represents the wave function

\[
\Psi = \mathcal{P}_{LLL} A \left[ z_1^N \cdot \prod_{i=2}^N z_i^{-2} \right] \Phi_{1}^{2p}. \tag{8}
\]

This state has been interpreted as a charged quasiparticle excitation of the \( \nu = 1/(2p + 1) \) FQHE state. The \([N - 2, 2]\) state (Fig. 1(c)) occurs at \( L = (2p + 1)N(N - 1)/2 - 2(N - 1) \), and has the wave function

\[
\Psi = \mathcal{P}_{LLL} A \left[ z_1^3 \cdot z_2^6 \cdot \prod_{i=3}^N z_i^{-3} \right] \Phi_{1}^{2p}. \tag{9}
\]

For many angular momenta, the basis contains more than one state. For six composite fermions at \( L = 33 \) we have two compact states \([3,3]\) and \([4,1,1]\), as depicted schematically in Fig. 2(a). The basis functions are given by

\[
\Psi_{1}^{L=33} = \mathcal{P}_{LLL} A \left[ \prod_{i=1}^3 \left( z_i^* z_i^{-1} \right) \cdot \prod_{i=4}^6 z_i^{-4} \right] \Phi_{1}^2, \tag{10a}
\]

\[
\Psi_{2}^{L=33} = \mathcal{P}_{LLL} A \left[ \prod_{i=3}^6 z_i^{-3} \right] \Phi_{1}^2. \tag{10b}
\]

These have the same CF kinetic energy, leading to \( D^* = 2 \) at \( L = 33 \). The five basis states at \( L = 34 \) are shown in Fig. 2(b), derived from either \([4,1,1]\) or \([3,3]\) by increasing the angular momentum by one unit. The corresponding basis functions are written as

\[
\Psi_{1}^{L=34} = \mathcal{P}_{LLL} A \left[ \eta_1^{-1}(z_1) \cdot \eta_1^0(z_2) \cdot \eta_1^{0}(z_3) \cdot \eta_0^{0}(z_4) \cdot \eta_0^{0}(z_5) \cdot \eta_0^{0}(z_6) \right] \Phi_{1}^2, \tag{11a}
\]

\[
\Psi_{2}^{L=34} = \mathcal{P}_{LLL} A \left[ \eta_1^{-1}(z_1) \cdot \eta_1^{0}(z_2) \cdot \eta_1^{0}(z_3) \cdot \eta_0^{0}(z_4) \cdot \eta_1^{0}(z_5) \cdot \eta_0^{0}(z_6) \right] \Phi_{1}^2, \tag{11b}
\]

\[
\Psi_{3}^{L=34} = \mathcal{P}_{LLL} A \left[ \eta_2^{-2}(z_1) \cdot \eta_1^{-1}(z_2) \cdot \eta_0^{0}(z_3) \cdot \eta_0^{0}(z_4) \cdot \eta_0^{0}(z_5) \cdot \eta_0^{0}(z_6) \right] \Phi_{1}^2, \tag{11c}
\]

\[
\Psi_{4}^{L=34} = \mathcal{P}_{LLL} A \left[ \eta_2^{-2}(z_1) \cdot \eta_1^{-1}(z_2) \cdot \eta_0^{0}(z_3) \cdot \eta_0^{0}(z_4) \cdot \eta_0^{0}(z_5) \cdot \eta_0^{0}(z_6) \right] \Phi_{1}^2, \tag{11d}
\]

\[
\Psi_{5}^{L=34} = \mathcal{P}_{LLL} A \left[ \eta_2^{-2}(z_1) \cdot \eta_1^{-1}(z_2) \cdot \eta_0^{0}(z_3) \cdot \eta_0^{0}(z_4) \cdot \eta_0^{0}(z_5) \cdot \eta_0^{0}(z_6) \right] \Phi_{1}^2. \tag{11e}
\]

Here

\[
\eta_n^{l}(z) \equiv z^l L_n^l (zz^*/2) \tag{12}
\]

with \( L_n^l(x) \) being an associated Laguerre polynomial.

The projection into the lowest LL is accomplished by the method outlined in the literature. To give a simple example, consider the state \([N - 1, 1]\) state in Eq. 8. We use the identity (apart from the constant factor),

\[
A \left[ z_1^* \cdot \prod_{i=2}^N z_i^{-2} \right] \prod_{j<k} (z_j - z_k)^{2p} = A \left[ z_1^* J_p^* \cdot \prod_{i=2}^N (z_i^{-2} J_{p_i}^*) \right] \tag{13}
\]
TABLE I: Comparison between the CF and the exact energies (V_{CF} and V_{ex}) for N = 4. The symbols in this and the following tables are defined in the text. The CF energy is given by Equation (15).

| L | D | D^* | V_{CF} | L | D | D^* | V_{CF} | L | D | D^* | V_{CF} |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 5 | 1 | 1.8759 | 1.8748 | 26 | 11 | 6320 | 4.6181 | 4.6181 | 24 | 11 | 6320 | 4.6181 | 4.6181 |
| 6 | 1 | 1.8759 | 1.8748 | 27 | 12 | 6420 | 4.6181 | 4.6181 | 25 | 12 | 6420 | 4.6181 | 4.6181 |
| 7 | 1 | 1.8759 | 1.8748 | 28 | 13 | 6420 | 4.6181 | 4.6181 | 26 | 13 | 6420 | 4.6181 | 4.6181 |
| 8 | 1 | 1.8759 | 1.8748 | 29 | 14 | 6420 | 4.6181 | 4.6181 | 27 | 14 | 6420 | 4.6181 | 4.6181 |
| 9 | 1 | 1.8759 | 1.8748 | 30 | 15 | 6420 | 4.6181 | 4.6181 | 28 | 15 | 6420 | 4.6181 | 4.6181 |

TABLE II: Comparison between the CF and the exact energies (V_{CF} and V_{ex}) for N = 5.

| L | D | D^* | V_{CF} | L | D | D^* | V_{CF} | L | D | D^* | V_{CF} |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 7.0000 | 6.9983 | 31 | 1 | 6.6800 | 6.6783 | 32 | 1 | 6.6800 | 6.6783 |
| 11 | 1 | 7.0000 | 6.9983 | 33 | 1 | 6.6800 | 6.6783 | 34 | 1 | 6.6800 | 6.6783 |
| 12 | 1 | 7.0000 | 6.9983 | 35 | 1 | 6.6800 | 6.6783 | 36 | 1 | 6.6800 | 6.6783 |
| 13 | 1 | 7.0000 | 6.9983 | 37 | 1 | 6.6800 | 6.6783 | 38 | 1 | 6.6800 | 6.6783 |
| 14 | 1 | 7.0000 | 6.9983 | 39 | 1 | 6.6800 | 6.6783 | 40 | 1 | 6.6800 | 6.6783 |
| 15 | 1 | 7.0000 | 6.9983 | 41 | 1 | 6.6800 | 6.6783 | 42 | 1 | 6.6800 | 6.6783 |
| 16 | 1 | 7.0000 | 6.9983 | 43 | 1 | 6.6800 | 6.6783 | 44 | 1 | 6.6800 | 6.6783 |
| 17 | 1 | 7.0000 | 6.9983 | 45 | 1 | 6.6800 | 6.6783 | 46 | 1 | 6.6800 | 6.6783 |

\[ \Psi \equiv e^{-\sum_{i=1}^{N} \frac{|z_i|^2}{2} A} P_{LLL}(z_j^* J_P^0) \prod_{i=2}^{N} P_{LLL}(z_j^{2-2} J_P^0) \]

The final step is achieved by placing all of the z_j's to the
TABLE III: Comparison between the CF and the exact energies ($V_{\text{CF}}$ and $V_{\text{ex}}$) for $N = 6$.

| $L$ | $D^* V_{\text{ex}}$ | $V_{\text{CF}}$ | $L$ | $D^* V_{\text{ex}}$ | $V_{\text{CF}}$ | $L$ | $D^* V_{\text{ex}}$ | $V_{\text{CF}}$ |
|-----|---------------------|----------------|-----|---------------------|----------------|-----|---------------------|----------------|
| 19  | 5                   | 4.32568        | 19  | 5                   | 4.32568        | 19  | 5                   | 4.35268        |
| 20  | 7                   | 4.39138        | 20  | 7                   | 4.39138        | 20  | 7                   | 4.40302        |
| 21  | 11                  | 4.26439        | 21  | 11                  | 4.26439        | 21  | 11                  | 4.27635        |
| 22  | 14                  | 4.26453        | 22  | 14                  | 4.26453        | 22  | 14                  | 4.27657        |
| 23  | 20                  | 4.15579        | 23  | 20                  | 4.15579        | 23  | 20                  | 4.16253        |
| 24  | 26                  | 4.05541        | 24  | 26                  | 4.05541        | 24  | 26                  | 4.06188        |
| 25  | 35                  | 3.92152        | 25  | 35                  | 3.92152        | 25  | 35                  | 3.92355        |
| 26  | 44                  | 3.90707        | 26  | 44                  | 3.90707        | 26  | 44                  | 3.90868        |
| 27  | 58                  | 3.79370        | 27  | 58                  | 3.79370        | 27  | 58                  | 3.79420        |
| 28  | 71                  | 3.79370        | 28  | 71                  | 3.79370        | 28  | 71                  | 3.79420        |
| 29  | 90                  | 3.69049        | 29  | 90                  | 3.69049        | 29  | 90                  | 3.69209        |
| 30  | 110                 | 3.57619        | 30  | 110                 | 3.57619        | 30  | 110                 | 3.57824        |
| 31  | 136                 | 3.56264        | 31  | 136                 | 3.56264        | 31  | 136                 | 3.56460        |
| 32  | 163                 | 3.53239        | 32  | 163                 | 3.53239        | 32  | 163                 | 3.53413        |
| 33  | 199                 | 3.41858        | 33  | 199                 | 3.41858        | 33  | 199                 | 3.42012        |
| 34  | 235                 | 3.40435        | 34  | 235                 | 3.40435        | 34  | 235                 | 3.40591        |
| 35  | 282                 | 3.28942        | 35  | 282                 | 3.28942        | 35  | 282                 | 3.29019        |
| 36  | 331                 | 3.28587        | 36  | 331                 | 3.28587        | 36  | 331                 | 3.28654        |
| 37  | 391                 | 3.26718        | 37  | 391                 | 3.26718        | 37  | 391                 | 3.26781        |
| 38  | 454                 | 3.21604        | 38  | 454                 | 3.21604        | 38  | 454                 | 3.21662        |
| 39  | 532                 | 3.11031        | 39  | 532                 | 3.11031        | 39  | 532                 | 3.11082        |
| 40  | 612                 | 3.08646        | 40  | 612                 | 3.08646        | 40  | 612                 | 3.08707        |
| 41  | 709                 | 3.06846        | 41  | 709                 | 3.06846        | 41  | 709                 | 3.06893        |
| 42  | 811                 | 3.03681        | 42  | 811                 | 3.03681        | 42  | 811                 | 3.03728        |
| 43  | 931                 | 3.00162        | 43  | 931                 | 3.00162        | 43  | 931                 | 3.00208        |
| 44  | 1057                | 2.95620        | 44  | 1057                | 2.95620        | 44  | 1057                | 2.95664        |
| 45  | 1206                | 2.86015        | 45  | 1206                | 2.86015        | 45  | 1206                | 2.86059        |
| 46  | 1360                | 2.86015        | 46  | 1360                | 2.86015        | 46  | 1360                | 2.86059        |
| 47  | 1540                | 2.83682        | 47  | 1540                | 2.83682        | 47  | 1540                | 2.83726        |
| 48  | 1729                | 2.80401        | 48  | 1729                | 2.80401        | 48  | 1729                | 2.80445        |
| 49  | 1945                | 2.76617        | 49  | 1945                | 2.76617        | 49  | 1945                | 2.76651        |
| 50  | 2172                | 2.71674        | 50  | 2172                | 2.71674        | 50  | 2172                | 2.71708        |
| 51  | 2432                | 2.69635        | 51  | 2432                | 2.69635        | 51  | 2432                | 2.69668        |

Left, and substituting $\partial^2/\partial z_j^2$ into $z_j^*$ with the assumption that the derivatives do not act on the Gaussian factor. The resulting wave function is then given by

$$\Psi = A \left[ \sum_{j \neq l} \frac{1}{z_i - z_j} \prod_{i=2}^{N} (z_i - z_j)^{-2} \right] \Phi^{2p}_1. \quad (16)$$

Lowest LL projection of other can be accomplished similarly, although the details are more complicated.

III. NUMERICAL METHODS

A. Exact diagonalization

We calculate the exact interaction energy for small systems by either numerical diagonalization using standard routines for small $L$, or a modified Lanczos algorithm for larger $L$. In either cases, it is essential to know the Coulomb matrix elements. In the second quantization language, the Coulomb Hamiltonian is written as

$$H = \frac{1}{2} \sum_{r,s,t,u} (r,s|V|t,u) a_r^+ a_s^+ a_t a_u,$$  \quad (17)

where the operator $a_r^+ (a_r)$ creates (annihilates) a particle at state $|r\rangle$ with angular momentum $V$. Is the Coulomb interaction in real space and $(r,s|V|t,u)$ is its restriction to the lowest Landau level Hilbert space. Several expressions for $(r,s|V|t,u)$ exist in the literature.

In this work we use the formula derived by Tsiper.

Each term in the sum on the right hand side of Eq. (15) is positive definite, which makes this expression more stable in numerical calculations, which is especially important.
TABLE IV: Comparison between the CF and the exact energies ($V_{CF}$ and $V_{ex}$) for $N = 7$.

| L   | D | D* | $V_{CF}$ | L   | D | D* | $V_{CF}$ | L   | D | D* | $V_{CF}$ | L   | D | D* | $V_{CF}$ |
|-----|---|----|----------|-----|---|----|----------|-----|---|----|----------|-----|---|----|----------|
| 26  | 7 | D* | V_{CF}   | 27  | 8 | D* | V_{CF}   | 28  | 9 | D* | V_{CF}   | 29  | 10| D* | V_{CF}   |
| 27  | 11| D* | V_{CF}   | 28  | 12| D* | V_{CF}   | 29  | 13| D* | V_{CF}   | 30  | 14| D* | V_{CF}   |
| 28  | 15| D* | V_{CF}   | 29  | 16| D* | V_{CF}   | 30  | 17| D* | V_{CF}   | 31  | 18| D* | V_{CF}   |
| 29  | 19| D* | V_{CF}   | 30  | 20| D* | V_{CF}   | 31  | 21| D* | V_{CF}   | 32  | 22| D* | V_{CF}   |
| 30  | 23| D* | V_{CF}   | 31  | 24| D* | V_{CF}   | 32  | 25| D* | V_{CF}   | 33  | 26| D* | V_{CF}   |
| 31  | 27| D* | V_{CF}   | 32  | 28| D* | V_{CF}   | 33  | 29| D* | V_{CF}   | 34  | 30| D* | V_{CF}   |
| 32  | 31| D* | V_{CF}   | 33  | 32| D* | V_{CF}   | 34  | 33| D* | V_{CF}   | 35  | 34| D* | V_{CF}   |
| 33  | 35| D* | V_{CF}   | 34  | 36| D* | V_{CF}   | 35  | 37| D* | V_{CF}   | 36  | 38| D* | V_{CF}   |

TABLE V: Comparison between the CF and the exact energies ($V_{CF}$ and $V_{ex}$) for $N = 8$.

| L   | D | D* | $V_{CF}$ | L   | D | D* | $V_{CF}$ | L   | D | D* | $V_{CF}$ | L   | D | D* | $V_{CF}$ |
|-----|---|----|----------|-----|---|----|----------|-----|---|----|----------|-----|---|----|----------|
| 34  | 1 | D* | V_{CF}   | 35  | 2 | D* | V_{CF}   | 36  | 3 | D* | V_{CF}   | 37  | 4 | D* | V_{CF}   |
| 35  | 5 | D* | V_{CF}   | 36  | 6 | D* | V_{CF}   | 37  | 7 | D* | V_{CF}   | 38  | 8 | D* | V_{CF}   |
| 36  | 9 | D* | V_{CF}   | 37  | 10| D* | V_{CF}   | 38  | 11| D* | V_{CF}   | 39  | 12| D* | V_{CF}   |
| 37  | 13| D* | V_{CF}   | 38  | 14| D* | V_{CF}   | 39  | 15| D* | V_{CF}   | 40  | 16| D* | V_{CF}   |
| 38  | 17| D* | V_{CF}   | 39  | 18| D* | V_{CF}   | 40  | 19| D* | V_{CF}   | 41  | 20| D* | V_{CF}   |
| 39  | 21| D* | V_{CF}   | 40  | 22| D* | V_{CF}   | 41  | 23| D* | V_{CF}   | 42  | 24| D* | V_{CF}   |
| 40  | 25| D* | V_{CF}   | 41  | 26| D* | V_{CF}   | 42  | 27| D* | V_{CF}   | 43  | 28| D* | V_{CF}   |
| 41  | 29| D* | V_{CF}   | 42  | 30| D* | V_{CF}   | 43  | 31| D* | V_{CF}   | 44  | 32| D* | V_{CF}   |

for large $L$. 

Exact numerical diagonalization is limited to systems with small numbers of particles at small angular momentum $L$, because the size of the Hilbert space grows exponentially fast with $N$ and for $L$. For example, for $N = 6$, the Fock space dimension grows from 21 to 701661 as $L$ is increased from 21 to 148. When $D$ becomes large, we have obtained the ground state energy using the modified Lanczos algorithm of Gagliano et al. 31 Briefly, the algorithm begins with an initial guess of the ground state $|\psi_0\rangle$. By applying the Hamiltonian $H$ onto $|\psi_0\rangle$, a new state $|\psi_1\rangle$ is defined as the following

$$|\psi_1\rangle = \frac{H|\psi_0\rangle - \langle H|\psi_0\rangle}{\sqrt{\langle H^2 \rangle - \langle H \rangle^2}},$$

where the notation $\langle H \rangle$ represents the expectation value $\langle \psi_0 | H | \psi_0 \rangle$. It is straightforward to verify that $|\psi_1\rangle$ is normalized and orthogonal to $|\psi_0\rangle$ by this construction. The Hamiltonian $H$ is now diagonalized in the subspace spanned by $|\psi_0\rangle, |\psi_1\rangle$, and the lowest eigenvalue $\varepsilon$ and its corresponding eigenvector $|\psi_1\rangle$ are chosen as a better approximation to the true ground state and its energy than $H$ and $|\psi_0\rangle$. In terms of $\langle H \rangle$ and $|\psi_0\rangle$, the “better” ground state energy and corresponding state can be written as

$$\varepsilon = \langle H \rangle + \alpha \varepsilon,$$

$$|\psi_0\rangle = \frac{|\psi_0\rangle + \alpha |\psi_1\rangle}{\sqrt{1 + \alpha^2}}.$$
TABLE VI: Comparison between the CF and the exact energies (V\text{CF} and Vex) for N = 9.

| L | D | D* | Vex | V\text{CF} | L | D | D* | Vex | V\text{CF} |
|---|---|---|---|---|---|---|---|---|---|---|
| 50 | 6 | 51.9063 | 51.9062(20) | 66 | 653 | 6 | 10.4788 | 10.4811(27) |
| 51 | 11 | 51.8667 | 51.8669(24) | 67 | 807 | 5 | 10.4256 | 10.4327(6) |
| 52 | 15 | 51.7534 | 51.7551(12) | 68 | 984 | 5 | 10.3294 | 10.3375(11) |
| 53 | 22 | 51.6444 | 51.6565(8) | 69 | 1204 | 5 | 10.2240 | 10.2322(23) |
| 54 | 30 | 51.5378 | 51.5388(15) | 70 | 1455 | 5 | 10.2240 | 10.2322(42) |
| 55 | 42 | 51.4332 | 51.4328(8) | 71 | 1761 | 5 | 10.1458 | 10.1473(16) |
| 56 | 55 | 51.2470 | 51.2473(33) | 72 | 2112 | 5 | 10.0508 | 10.0564(6) |
| 57 | 75 | 51.0310 | 51.0310(9) | 73 | 2534 | 5 | 9.9478 | 9.9625(15) |
| 58 | 97 | 51.0244 | 51.0244(25) | 74 | 3015 | 5 | 9.9478 | 9.9545(12) |
| 59 | 128 | 50.9855 | 50.9864(15) | 75 | 3590 | 5 | 9.8653 | 9.8679(14) |
| 60 | 164 | 50.9979 | 50.9902(14) | 76 | 4242 | 5 | 9.7660 | 9.7782(17) |
| 61 | 212 | 50.8987 | 50.8985(11) | 77 | 5013 | 5 | 9.6703 | 9.6807(8) |
| 62 | 267 | 50.8122 | 50.8124(27) | 78 | 5888 | 5 | 9.5603 | 9.6183(15) |
| 63 | 340 | 50.7207 | 50.7222(13) | 79 | 6912 | 5 | 9.5092 | 9.6085(20) |
| 64 | 423 | 50.6750 | 50.6751(36) | 80 | 8070 | 5 | 9.5093 | 9.5225(7) |
| 65 | 530 | 50.5949 | 50.5976(40) | 81 | 9418 | 5 | 9.4836 | 9.4948(21) |

TABLE VII: Comparison between the CF and the exact energies (V\text{CF} and Vex) for N = 10.

in which

\begin{equation}
\alpha = f - \sqrt{f^2 + 1},
\end{equation}

\begin{equation}
f = \frac{1}{2} (\langle H \rangle^2 - 3|\langle H \rangle|^2 + 2 |\langle H \rangle|^3),
\end{equation}

\begin{equation}
b = \sqrt{\langle H^2 \rangle} - |\langle H \rangle|.
\end{equation}

The state |ψ_0\rangle is then used as a new initial guess and the entire procedure is iterated until the relative energy difference |\varepsilon - |\langle H \rangle| \rangle is smaller than a predefined tolerance.

We place the program on a node of a Beowulf type PC cluster, each node consists a dual PentiumIII 1GHz processor. The modified Lanczos algorithm converges relatively fast to the true state. For example, when N = 6 it takes approximately 24 CPU hours to obtain the ground state energy for L = 135. The largest system we have studied by the Lanczos method has a Fock space dimension of 81779. We note that for large L, our energies are slightly lower than those in Ref.15, presumably because they work with a truncated basis.

B. CF diagonalization

CF diagonalization refers to a diagonalization of the full Coulomb Hamiltonian in a correlated CF basis. The basis wave functions correspond to states with low "CF kinetic energies" (the kinetic energy is given by \( \sim \sum_{j=1}^{N} n_j \)) with the restriction that the total angular momentum is \( L \), i.e.,

\begin{equation}
\sum_{j=1}^{N} l_j + p(N - 1) = L,
\end{equation}

where \( n_j \) and \( l_j \) are the A-level and the angular momentum indices, respectively, for composite fermions. In most of this paper, we choose states that have the lowest CF kinetic energy (zeroth order CF diagonalization). By allowing hybridization with CF states with higher kinetic energies (higher order CF diagonalization), more accurate approximations can be obtained, as seen explicitly below. As illustrated in the previous section, the wave function \( \Psi_L \) corresponding to the basis at \( L \) is then
The exact interaction energy (circle) vs. the mean-field CF ground-state energy (square) as a function of the angular momentum $L$ for $N=6$. The exact energy is plotted in units of $e^2/\epsilon \ell$ while the CF energy is in arbitrary units.

given by

$$\Psi^L_\alpha = A \left[ \psi_{n_1}^{(\alpha)} j_1^{(\alpha)}(z_1) \cdot \psi_{n_2}^{(\alpha)} j_2^{(\alpha)}(z_2) \cdots \psi_{n_N}^{(\alpha)} j_N^{(\alpha)}(z_N) \right] \times \Phi_1^{2p}, \quad (\alpha = 1, 2, \ldots, D^*) \tag{27}$$

where

$$\psi_{n_i}(z_i) \equiv J^{-p}_{i1} P_{LLL}[\eta_i(z_i) J_1^p]. \tag{28}$$

The CF basis states $\Psi^L_\alpha$ constructed in this manner are not orthogonal to one another at given $L$, and sometimes not even linearly independent. We use Gram-Schmidt procedure to orthogonalize the states. The orthogonal basis states $|\xi\rangle$ are expressed as

$$|\xi_\alpha\rangle = |\eta_\alpha\rangle - \sum_{\gamma=1}^{\alpha-1} \frac{\langle \xi_\alpha | \eta_\alpha \rangle}{\langle \xi_\gamma | \xi_\gamma \rangle} |\xi_\gamma\rangle, \tag{29}$$

FIG. 3: The relative errors of CF ground-state energy compared with the exact energies for (a) $N=4$; (b) $N=5$; (c) $N=6$; (d) $N=7$. 
FIG. 5: The exact interaction energies $V$ (dashes) are given as a function of the angular momentum $L$ for (a) $N = 4$ (b) $N = 6$ particles. The dots are the predictions of the zeroth-order CF theory. Different panels correspond to $L$ regions where composite fermions of different flavors are relevant. The energies are quoted in units of $e^2/\epsilon \ell$.

where the normalized state $|\eta_{\alpha}\rangle$ is defined by

$$|\eta_{\alpha}\rangle \equiv \frac{|\Psi_{\alpha}\rangle}{\sqrt{\langle \Psi_{\alpha}|\Psi_{\alpha}\rangle}}.$$  

(30)

From the relation in Eq. (29) we can find the recursion relation for the transformation matrix $U_{\alpha\beta}$, defined by

$$U_{\alpha\beta} = \begin{cases} 
- \sum_{\gamma=1}^{\alpha-1} \sum_{\delta=1}^{\gamma} U_{\gamma\delta}^{*} O_{\delta\alpha} U_{\gamma\beta} & \text{for } \beta < \alpha, \\
1 & \text{for } \beta = \alpha, \\
0 & \text{for } \beta > \alpha, 
\end{cases}$$

(31)

where $O_{\alpha\beta} \equiv \langle \eta_{\alpha} | \eta_{\beta}\rangle$. The computation of $U_{\alpha\beta}$ enables us to calculate the Coulomb Hamiltonian matrix.
elements $V_{\alpha\beta}$ in orthonormal basis sets,

$$V_{\alpha\beta} = \frac{\langle \xi_\alpha|V|\xi_\beta \rangle}{\sqrt{\langle \xi_\alpha|\xi_\alpha \rangle \langle \xi_\beta|\xi_\beta \rangle}},$$

where

$$\langle \xi_\alpha|V|\xi_\beta \rangle = \sum_{\gamma,\delta} U_{\alpha\gamma}^* U_{\beta\delta} \langle \eta_\gamma|V|\eta_\delta \rangle,$$

$$\langle \xi_\alpha|\xi_\alpha \rangle = \sum_{\gamma,\delta} U_{\alpha\gamma}^* U_{\beta\delta} \mathcal{O}_{\gamma\delta}.$$

The Coulomb Hamiltonian matrix in Eq. (32) is diagonalized to obtain the energy and the wave function of the ground state in the CF theory.

Based on the CF diagonalization procedure described in Sec. III B we have computed the CF ground state energies as a function of total angular momentum $L$ for $N = 6$. For small angular momenta the mean-field CF model predicts correctly the positions of cusps on ground-state energy (e.g., see Fig. 3(a)). However, with increasing $L$, it gradually fails to capture the correct positions of cusp states. Such discrepancies between the exact results and the mean-field predictions motivate the need for an investigation of the residual interactions between composite fermions, considered in the subsequent sections.

IV. MEAN-FIELD MODEL

It is customary to first consider the mean-field version of CF model, in which the interaction between composite fermions is assumed to vanish. Then the interaction energy of electron systems is completely transformed into the “kinetic energy” of composite fermions, and can be evaluated in units of CF cyclotron energy $\hbar \omega^*$ by summing the $A$-level indices of all occupied CF states

$$V_{\text{CF-MF}} = \left( \sum_{j=1}^{N} n_j \right) \hbar \omega^*.$$

Figure 3 compares the interaction energies predicted by the mean-field CF theory with the exact ground-state energies as a function of total angular momentum $L$ for $N = 6$. For small angular momenta the mean-field CF model predicts correctly the positions of cusps on ground-state energy (e.g., see Fig. 3(a)). However, with increasing $L$, it gradually fails to capture the correct positions of cusp states. Such discrepancies between the exact results and the mean-field predictions motivate the need for an investigation of the residual interactions between composite fermions, considered in the subsequent sections.

V. ZERO-ORDER COMPOSITE FERMION THEORY

Based on the CF diagonalization procedure described in Sec. III B we have computed the CF ground state energies at the zeroth order, i.e. by including only the lowest kinetic energy CF basis states. We have also carried out exact diagonalization for $N \leq 10$. It is possible to go to arbitrarily large values of $L$ within the CF theory, but available computer memory and execution time restricts our exact diagonalization study to $L \leq 148$, 127, 118, 116, and 113 for $N = 6$, 7, 8, 9, and 10, respectively. (To our knowledge, the largest systems for which exact results have been computed are $N = 8$, $L = 140$ with $D_{\text{ex}} = 3023010$ and $N = 10$, $L = 135$ with $D_{\text{ex}} = 2977866$.) The results are listed in Tables I-VII which show that the CF energies compare well to the exact ones. (Many of the exact energies have been reported previously in the literature, but are included here for completeness.)

The deviation between the CF and the exact energies ($V_{\text{CF}}$ and $V_{\text{ex}}$) is $L$ dependent but small in the entire range of $L$ studied in this work. The largest deviations are 1.1% ($L = 36, N = 4$), 0.6% ($L = 102, N = 5$), 0.5% ($L = 135, N = 6$), 0.7% ($L = 112, N = 7$), 0.9% ($L = 89, N = 8$), 1.3% ($L = 114, N = 9$), and 0.2% ($L = 80, N = 10$). For $N = 4$, the maximum deviation occurs for composite fermions carrying 6-8 vortices; for $N \geq 5$, the deviation grows generally with $L$ in the range considered in this work (see Fig. 4).

The plot of interaction energy as a function of $L$ in Fig. 3 gives a demonstration of the accuracy of the CF predictions. In addition to the quantitative accuracy, the
qualitative features of the energy versus $L$ plot are reproduced faithfully by the CF theory. For $N = 4$, the major cusps occurs at $L = 4n + 2$. The system with six particles exhibits more complicated features. For system of $^2$CFs (top panel) shows cusps at $L = 21, 25, 27, 30, 33, 35, 39, 40$ and 45. As the flavor increases, the cusps at angular momenta other than $L = 5n$ become less prominent and eventually disappear. Such periodic behavior is consistent with the geometric interpretation.\textsuperscript{15,16}

VI. NEXT ORDER CF THEORY

The CF theory allows a systematic perturbative way of improving the results. Above we considered only the CF states with the lowest CF kinetic energy, called the zeroth-order CF theory. The next step is to include states with one more unit of the kinetic energy in the CF basis.\textsuperscript{31} The degree of improvement can be seen in Figs. 6, 7, and 8. Figure 6 shows the full spectrum for six electrons in a range of angular momentum; Figure 7 shows the spectrum from the zeroth order CF diagonalization,
and Fig. 8 from the first order. Both the zeroth and first order spectra capture the qualitative behavior and the positions of the cusps, but the first order theory is quantitatively much more accurate. In both cases, the discrepancy between the CF and the exact energies (\( V_{\text{CF}} \) and \( V_{\text{ex}} \)) grows with \( L \), because while the dimension of the CF basis remains the same when \( L \) is changed by \( N(N-1) \), the dimension of the full lowest LL Fock space increases rapidly. In spite of the small basis (which sometimes contains only one state at the zeroth order), the CF theory is quantitatively satisfactory.

VII. CONCLUDING REMARKS

Several authors\(^{12,15} \) have noted that the CF theory fails to produce the cusp positions for large \( L \). These comparisons, however, refer only to the mean-field model of composite fermions, in which the interaction energy of electrons at \( L \) is viewed as the kinetic energy of free fermions at an effective angular momentum \( L^* \), with the cyclotron energy treated as a parameter. The validity of the CF theory should not be confused with the validity of the mean-field picture, which serves, at best, as a useful guide; given its crudeness, it is in fact surprising it works as well as it does. A more substantive, microscopic test of the CF theory requires working with the correlated wave functions produced by the CF theory.

Our extensive study of quantum dot states shows that the microscopic composite fermion theory, defined through wave functions, gives an excellent description in regions including both liquid-like and crystal-like ground states, and continues to be satisfactory from very low angular momenta to the largest angular momenta studied to date. It provides an accurate approximation for the ground state wave function and the ground state energy at every single \( L \) in the wide range studied, and correctly reproduces all cusps in plot of the ground state energy vs. \( L \). Taken together, these results constitute a detailed verification for the validity of the composite fermion theory for quantum dots.

It is expected, from general considerations, that the ground state at large \( L \) will resemble a classical crystal, because large \( L \) implies small density (or small filling factor) with particles far from one another, as a result of which the system behaves more or less classically. Reference \(^{15} \) has studied a Hartree-Fock crystal trial wave function based on an analogy to the classical crystal ground state in a quantum dot. No crystalline correlations are put in by hand in our calculations described above, however. As implied by the successful comparisons with the exact results, and also confirmed by an explicit calculation of the pair correlation function\(^ {12,15} \), the CF theory automatically generates a crystal of correct symmetry. The CF approach offers many other advantages over the Hartree-Fock electron crystal description. The latter obtains wave functions and energies only for certain special values of \( L \), and even then only for the ground state. The CF theory, on the other hand, provides a quantitative understanding of states at all \( L \). For \( N = 6 \), Reference \(^{15} \) explicitly quotes energies from their approach for seven values of \( L \) in the range \( 75 \leq L \leq 135 \). For these angular momenta, the zeroth order CF theory gives lower energy in every case except at \( L = 135 \). (The state at \( L = 135 \) has one filled \( L \), described by the Laughlin wave function.) At the first order, the CF results improve substantially for large \( L \). As shown in Ref. \(^{15} \), an almost exact description of the crystallite at large \( L \) is obtained in terms of a crystal of composite fermions, wherein a combination of the crystal and CF physics are introduced right at the outset. It is gratifying that the principle that applies to the fractional quantum Hall effect in a bulk two-dimensional electron system also produces an understanding of the quantum dot physics at high magnetic fields.

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