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Analytical Theory of Strongly Correlated Wigner Crystals in the Lowest Landau Level

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In this work, we present an analytical theory of strongly correlated Wigner crystals (WCs) in the lowest Landau level (LLL) by constructing an approximate, but accurate effective two-body interaction for composite fermions (CFs) participating in the WCs. This requires integrating out the degrees of freedom of all surrounding CFs, which we accomplish analytically by approximating their wave functions by delta functions. This method produces energies of various strongly correlated WCs that are in excellent agreement with those obtained from the Monte Carlo simulation of the full CF crystal wave functions. We compute the compressibility of the strongly correlated WCs in the LLL and predict discontinuous changes at the phase boundaries separating different crystal phases.

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Wigner predicted more than eighty years ago [1] that, when the interaction energy is dominant over the kinetic energy, electrons form a crystal, which is called WC after its originator. One possible way of suppressing the kinetic energy relative to the interaction energy is via the application of a strong magnetic field to two-dimensional electron systems [2], which generates a fascinating series of various emergent quantum phases. The most celebrated examples are the fractional quantum Hall states [3], where new emergent quasiparticles called CFs form the quantum Hall liquid states [4, 5]. The quantum Hall liquid states are more effective in minimizing the interaction energy than WCs for a range of filling factors that is not too low. Nevertheless, WCs are expected to occur at sufficiently low filling factors. Indeed, insulating states observed at filling factor $\nu < 1/5$ are interpreted as pinned WCs [6–20]. More recently, indications of the existence of a WC in the LLL have been seen through commensurability magneto-resistance oscillations in bilayer Hall systems composed of a CF sea in one layer and a WC in the other [21].

Numerous theoretical studies have investigated the nature of WCs in the LLL [22–37]. Initially, Maki and Zotos [22] considered an uncorrelated Hartree-Fock WC of electrons, which was improved upon by Lam and Girvin [23] by incorporating correlations. In view of the success of the CF theory, Yi and Fertig [27] proposed a strongly correlated WC composed of CFs, which was subsequently shown by Chang *et al.* [33] to provide an accurate description at low filling factors ($\nu \leq 1/5$). Despite these extensive theoretical works, the calculation of a precise phase diagram of quantum Hall liquids versus CF crystals (CFCs) remained stalled for many years due to difficulties in obtaining the energy of CFCs in the thermodynamic limit accurately. This issue was resolved in a recent work [38] inspired by the Thomson problem [39]. Here, the CFC wave functions are constructed in the spherical geometry by placing the WC wave packet cen-

ters at the locations that minimize the Coulomb energy of N charged point particles on the surface of a sphere. Locally, these minimum energy positions resemble the hexagonal lattice, which is the minimum energy symmetry for a classical 2D electron crystal [40]. This allows a precise investigation of the CFC wave functions up to a fairly large system size ($N \sim 100$) [38].

The Monte Carlo (MC) simulation of the CFC wave functions is computationally quite expensive and rather difficult to implement. Furthermore, it turns out that even though the energy obtained from this method enables a determination of the phase diagram, it is not sufficiently accurate to allow an evaluation of quantities such as compressibility, which is related to the second derivative of the energy. We develop in this work an analytical theory of the CFCs by constructing an accurate effective two-body interaction, which is based on the two-body wave function of CFs participating in the CFCs. This requires integrating out the degrees of freedom of all surrounding CFs, which we accomplish analytically by approximating their wave functions as delta functions. We call this approach the “renormalized two-body formalism,” to be contrasted with the “isolated two-body formalism” where the effects of all surrounding CFs are neglected. The CFC energies obtained from the renormalized two-body formalism are in excellent agreement with those obtained from the MC simulation of the full CFC wave functions. With these analytical results, we obtain the compressibility and predict that its measurements, such as those carried out in GaAs heterostructures or in graphene [41–46], can detect the phase diagram of the CFCs.

We begin by constructing the wave function for the CFC carrying $2p$ vortices, or in short 2p CFC, as follows:

$$\Psi_{\nu}^{2p\text{CFC}} = \prod_{j < k} (z_j - z_k)^{2p} \Psi_{\nu^*}^{\text{MZ}}, \quad (1)$$

where $z_j = x_j + iy_j$ is the coordinates of the j -th electron. ν and ν^* denote the filling factors of electron and

CFCs, respectively. The function $\Psi_{\nu^*}^{\text{MZ}} = \text{Det}[\phi_{\mathbf{R}_i}(\mathbf{r}_j)]$ is the MZ wave function for the uncorrelated WC, comprising the LLL coherent-state wave function $\phi_{\mathbf{R}}(\mathbf{r}) = \frac{1}{\sqrt{2\pi}} \exp[-(\mathbf{r} - \mathbf{R})^2/4 - i(xY - yX)/2]$ centered at $\mathbf{R} = (X, Y)$ [22].

Without the Jastrow factor correlation, the energy of the uncorrelated Maki-Zotos (MZ) WC, i.e., ${}^0\text{CFC}$, can be computed from the effective two-body interaction [22]:

$$\begin{aligned} \frac{V^{\text{MZ}}(R_{ij})}{e^2/\epsilon l_B} &= \langle \psi^{{}^0\text{CFC}} | |\mathbf{r}_1 - \mathbf{r}_2|^{-1} | \psi^{{}^0\text{CFC}} \rangle \\ &= \frac{\sqrt{\pi}}{4} \text{sech}(R_{ij}^2/8) I_0(R_{ij}^2/8), \end{aligned} \quad (2)$$

where $R_{ij} = |\mathbf{R}_{ij}| = |\mathbf{R}_i - \mathbf{R}_j|$ is the distance between two crystal lattice centers. The uncorrelated two-body wave function is given by $\psi^{{}^0\text{CFC}}(\mathbf{r}_1, \mathbf{r}_2) = \mathcal{C}_0 \mathcal{A}[\phi_{\mathbf{R}_i}(\mathbf{r}_1)\phi_{\mathbf{R}_j}(\mathbf{r}_2)]$ with \mathcal{C}_0 being the normalization constant and \mathcal{A} being the antisymmetrization operator. I_0 is the modified Bessel function of the first kind. The energy per particle of the uncorrelated MZ WC, E^{MZ} , is computed by performing the Madelung-type lattice summation of the MZ effective two-body interaction energy between all pairs of electrons in the hexagonal lattice:

$$\frac{E^{\text{MZ}}}{e^2/\epsilon l_B} = \frac{1}{2N} \sum_{i \neq j} \left(\frac{V^{\text{MZ}}(R_{ij})}{e^2/\epsilon l_B} - \frac{1}{R_{ij}} \right) - \alpha \sqrt{\nu}, \quad (3)$$

where the terms $\frac{1}{2N} \sum_{i \neq j} \frac{1}{R_{ij}} + \alpha \sqrt{\nu}$ with $\alpha = 0.782133$ are subtracted to take into account the neutralizing effect of the uniform positive-charge background [40].

For strongly correlated WCs, we need to take care of the Jastrow factor. As a first try, we begin by focusing on two isolated CFs and ignoring all other surrounding CFs, in which situation the two-body CF wave function is obtained as $\psi_{\text{isol}}^{2p\text{CFC}}(\mathbf{r}_1, \mathbf{r}_2) = \mathcal{C}_{2p}(z_1 - z_2)^{2p} \mathcal{A}[\phi_{\mathbf{R}_i}(\mathbf{r}_1)\phi_{\mathbf{R}_j}(\mathbf{r}_2)]$. The normalization constant is $\mathcal{C}_{2p} = [{}_1F_1(2p+1; 1; R_{ij}^2/4) - {}_1F_1(2p+1; 1; -R_{ij}^2/4)]^{-1/2} / [\pi^{2p+1} \sqrt{2\Gamma(2p+1)} e^{-R_{ij}^2/8}]$ where ${}_1F_1(a; b; z) = \sum_{n=0}^{\infty} \frac{a^{(n)}}{b^{(n)} n!} z^n$ is the Kummer's hypergeometric function with $a^{(n)} = a(a+1)\cdots(a+n-1)$. We refer to this approach the isolated two-body formalism. Figure 1 (a) shows a schematic diagram for the isolated two-body formalism, which is accompanied by the probability density of the two-body CF wave function defined by $\rho_{\text{isol}}(\mathbf{r}) = \int d^2\mathbf{r}' |\psi_{\text{isol}}^{2p\text{CFC}}(\mathbf{r}, \mathbf{r}')|^2$ in Fig. 1 (c).

It is important to note that the actual distance between composite fermions d_{ij} is not exactly equal to the nominal distance R_{ij} , because the Jastrow factor incorporates an additional repulsion into the two-body wave function, pushing the wave packets slightly farther apart. To take this effect into account, we define d_{ij} to be the *median* distance between two maxima in the two-body probability density. Specifically, d_{ij} is related with R_{ij} so that $\frac{\partial}{\partial \mathbf{r}} |\psi_{\text{isol}}^{2p\text{CFC}}(\mathbf{r}_1, \mathbf{r}_2)|^2 = 0$ at $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 = (d_{ij}, 0)$

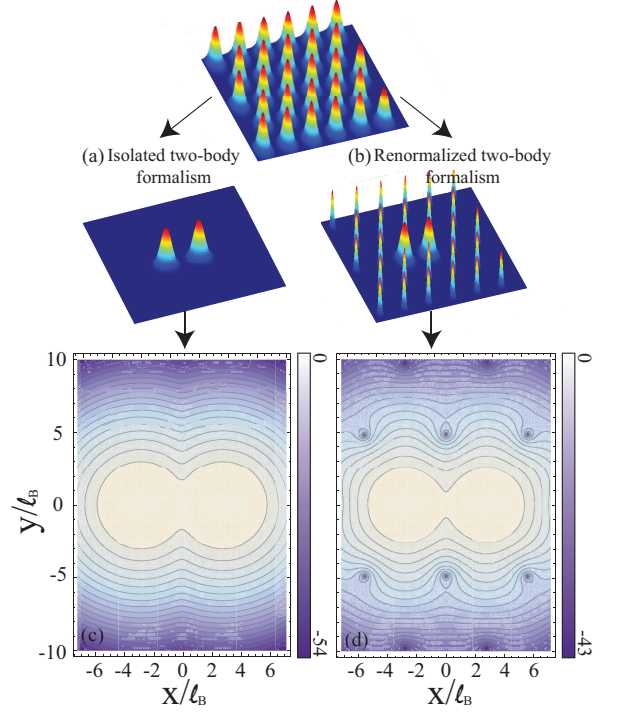


FIG. 1: (Color online) Schematic diagram showing (a) the isolated and (b) the renormalized two-body formalism, accompanied by the probability density of the two-body CF wave function in each formalism, (c) $\rho_{\text{isol}}(\mathbf{r}) = \int d^2\mathbf{r}' |\psi_{\text{isol}}^{2p\text{CFC}}(\mathbf{r}, \mathbf{r}')|^2$ and (d) $\rho_{\text{renorm}}(\mathbf{r}) = \int d^2\mathbf{r}' |\psi_{\text{renorm}}^{2p\text{CFC}}(\mathbf{r}, \mathbf{r}')|^2$, respectively. Here, we set $2p = 2$ and the nominal distance between crystal centers to be $6l_B$. Note that probability densities are plotted in the natural log scale.

with $\mathbf{R}_{ij} = (R_{ij}, 0)$, which, after some algebra, becomes $d_{ij}^2 - R_{ij}d_{ij} \coth(R_{ij}d_{ij}/4) - 8p = 0$. Note that d_{ij} is slightly larger than R_{ij} with their difference growing as $2p$ increases. Given this information, the effective two-body interaction between CFs in the isolated two-body formalism is computed as follows:

$$\begin{aligned} \frac{V_{\text{isol}}^{2p\text{CFC}}(d_{ij})}{e^2/\epsilon l_B} &= \langle \psi_{\text{isol}}^{2p\text{CFC}} | |\mathbf{r}_1 - \mathbf{r}_2|^{-1} | \psi_{\text{isol}}^{2p\text{CFC}} \rangle \\ &= \mathcal{B}_{2p} \frac{{}_1F_1(2p+1/2; 1; R_{ij}^2/4) - {}_1F_1(2p+1/2; 1; -R_{ij}^2/4)}{L_{2p}(-R_{ij}^2/4)e^{R_{ij}^2/4} - L_{2p}(R_{ij}^2/4)e^{-R_{ij}^2/4}} \end{aligned} \quad (4)$$

where $\mathcal{B}_{2p} = \Gamma(2p+1/2)/[2\Gamma(2p+1)]$ and $L_n(x)$ is the Laguerre polynomial. For the hexagonal lattice, d_{ij} is set equal to the distance between various crystal lattice centers via $d_{ij} = \sqrt{i^2a^2 + j^2b^2}$ with $a = (4\pi/\sqrt{3}\nu)^{1/2}$ and $b = \sqrt{3}a$.

In the isolated two-body formalism, the energy per particle of ${}^{2p}\text{CFC}$, $E_{\text{isol}}^{2p\text{CFC}}$, is evaluated similarly to Eq. (3) by replacing V^{MZ} with $V_{\text{isol}}^{2p\text{CFC}}$. Figure 2 (a) shows

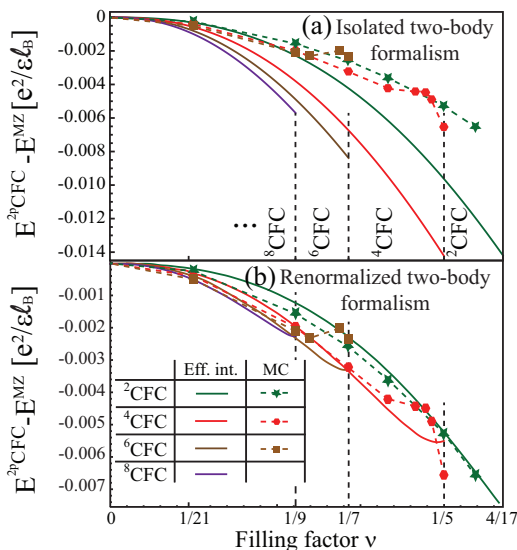


FIG. 2: (Color online) Energy per particle of various CFC states, $E^{2p\text{CFC}}$, in reference to that of the MZ WC, E^{MZ} , as a function of filling factor, ν , obtained in (a) the isolated and (b) the renormalized two-body formalism. Symbols and dashed lines are obtained from the MC simulation of the full CFC wave functions. Note that each $2p\text{CFC}$ is the lowest energy state (at least, among various CFC states) within the range of $1/(2p+3) < \nu \lesssim 1/(2p+1)$ for $2p \geq 2$. The MZ WC, or 0CFC is not energetically favorable at any filling factor ranges.

$E_{\text{isol}}^{2p\text{CFC}} - E^{\text{MZ}}$ as a function of filling factor, which is compared with the MC simulation results obtained from the full CF wave function in the spherical geometry. As one can see, $E_{\text{isol}}^{2p\text{CFC}} - E^{\text{MZ}}$ shows a reasonably good agreement with the MC simulation results, especially at low filling factors. There are, however, some sizable quantitative discrepancies in general.

To improve upon the isolated two-body formalism, it is necessary to include Jastrow-factor correlation effects arising from all surrounding CFs in some fashion. To this end, we test an approximation called *the surrounding delta-function approximation*, where the wave functions of all surrounding CFs are approximated as delta functions. See Fig. 1 (b) for a schematic diagram. This approximation should be exact in the limit of large separation between crystalline CFs. Within the surrounding delta-function approximation, one can integrate out the degrees of freedom of all surrounding CFs and then derive the analytical two-body CF wave function. For convenience, we call this approach the renormalized two-body formalism.

In the renormalized two-body formalism, the two-body CF wave function is written as $\psi_{\text{renorm}}^{2p\text{CFC}}(\mathbf{r}_1, \mathbf{r}_2) \propto \psi_{\text{isol}}^{2p\text{CFC}}(\mathbf{r}_1, \mathbf{r}_2) \prod_{k \neq i, j} (z_1 - Z_k)^{2p} \prod_{l \neq i, j} (z_2 - Z_l)^{2p}$, where Z_k denotes the coordinates of the k -th crystal lattice

center. After dividing a constant factor $\prod_{k \neq i, j} (Z_i - Z_k)^{2p} \prod_{l \neq i, j} (Z_j - Z_l)^{2p}$, The above equation can be rewritten as

$$\psi_{\text{renorm}}^{2p\text{CFC}}(\mathbf{r}_1, \mathbf{r}_2) = \tilde{\mathcal{C}}_{2p} (z_1 - z_2)^{2p} \times \mathcal{A} \left[\Gamma_{ij}^{2p}(\mathbf{r}_1, \mathbf{r}_2) \tilde{\phi}_{\mathbf{R}_i}(\mathbf{r}_1) \tilde{\phi}_{\mathbf{R}_j}(\mathbf{r}_2) \right], \quad (5)$$

where $\tilde{\mathcal{C}}_{2p}$ is the normalization constant, $\Gamma_{ij}^{2p}(\mathbf{r}_1, \mathbf{r}_2) = (Z_i - Z_j)^{4p} / [(z_1 - Z_j)^{2p} (z_2 - Z_i)^{2p}]$, and $\tilde{\phi}_{\mathbf{R}_i}(\mathbf{r}) = \phi_{\mathbf{R}_i}(\mathbf{r}) \prod_{k \neq i} \frac{(z - Z_k)^{2p}}{(Z_i - Z_k)^{2p}} \equiv \phi_{\mathbf{R}_i}(\mathbf{r}) [\mathcal{F}_{\mathbf{R}_i}(\mathbf{r})]^p$, which is the renormalized version of the coherent-state wave function centered at \mathbf{R}_i .

It is important to note that all the complicated many-body correlations are embedded in the renormalization factor $\mathcal{F}_{\mathbf{R}_i}(\mathbf{r})$. The success of this approach stems from the fact that we are able to obtain the analytical form of $\mathcal{F}_{\mathbf{R}_i}(\mathbf{r})$:

$$\mathcal{F}_{\mathbf{R}_i}(\mathbf{r}) = \frac{\theta_1\left(\frac{\pi}{a}(z - Z_i) \middle| i\frac{b}{a}\right) \theta_1\left(\frac{i\pi}{b}(z - Z_i) \middle| i\frac{a}{b}\right)}{i\frac{\pi^2}{ab} \theta_1'(0 \middle| i\frac{b}{a}) \theta_1'(0 \middle| i\frac{a}{b}) (z - Z_i)^2} \times \frac{\theta_3\left(\frac{\pi}{a}(z - Z_i) \middle| i\frac{b}{a}\right) \theta_3\left(\frac{i\pi}{b}(z - Z_i) \middle| i\frac{a}{b}\right)}{\theta_3(0 \middle| i\frac{b}{a}) \theta_3(0 \middle| i\frac{a}{b})}, \quad (6)$$

where $\theta_n(z|\tau)$ is the Jacobi theta function and $b = \sqrt{3}a$ with a being the lattice constant. See Supplementary Material for details. Figure 1 (d) shows the renormalized probability density defined by $\rho_{\text{renorm}}(\mathbf{r}) = \int d^2\mathbf{r}' |\psi_{\text{renorm}}^{2p\text{CFC}}(\mathbf{r}, \mathbf{r}')|^2$. As one can see, the renormalized probability density exhibits the hexagonal symmetry of the WC which was absent in the isolated two-body formalism.

As before, the energy per particle in the renormalized two-body formalism, $E_{\text{renorm}}^{2p\text{CFC}}$, can be computed as the Madelung-type lattice summation of the renormalized effective two-body interaction, $V_{\text{renorm}}^{2p\text{CFC}} / (e^2/\epsilon l_B) = \langle \psi_{\text{renorm}}^{2p\text{CFC}} | |\mathbf{r}_1 - \mathbf{r}_2|^{-1} | \psi_{\text{renorm}}^{2p\text{CFC}} \rangle$. Note that, in general, $V_{\text{renorm}}^{2p\text{CFC}}$ depends on the vector \mathbf{R}_{ij} , not just on the distance R_{ij} . Conveniently, however, $V_{\text{renorm}}^{2p\text{CFC}}$ can be well approximated as a function of only R_{ij} if $R_{ij} \gtrsim [4\pi(2p+1)/\sqrt{3}]^{1/2}$. Also, due to the additional repulsion from all surrounding CFs, the actual distance d_{ij} becomes quite close to the nominal distance R_{ij} in most situations so that R_{ij} can be simply regarded as d_{ij} .

Figure 2 (b) shows $E_{\text{renorm}}^{2p\text{CFC}} - E^{\text{MZ}}$ as a function of filling factor. As one can see, the results from the renormalized two-body formalism are in excellent agreement with those from the MC simulation of the full CFC wave functions. It is interesting to observe that the renormalized two-body formalism can even capture the initial upturn of the energy near $\nu = 1/(2p+1)$ for each corresponding $2p\text{CFC}$. The most significant discrepancy is that the MC results exhibit sharp drops immediately following such upturns. It is important to note, however, that, regardless of being isolated or renormalized, the

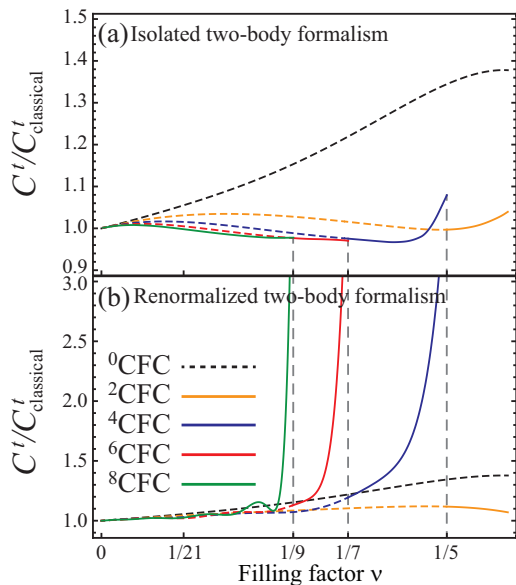


FIG. 3: (Color online) Shear modulus, C^t , of various CFC states as a function of filling factor, ν , obtained in (a) the isolated and (b) the renormalized two-body formalism. For convenience, C^t is expressed as its relative ratio with respect to that for the classical WC, $C_{\text{classical}}^t/(e^2/\ell_B) = 0.0978\sqrt{\nu}$. Note that C^t of each ^{2p}CFC is valid only within the range of $1/(2p+3) < \nu \lesssim 1/(2p+1)$, where its curve is plotted in a solid line, denoting that the ^{2p}CFC is the lowest energy state here.

two-body formalism for each ^{2p}CFC is supposed to lose its validity near $\nu = 1/(2p+1)$ since, here, wave packets are highly overlapping and thus higher-body corrections become important. Given the simplification in the two-body formalism, we consider the agreement to be excellent.

Bolstered by the quantitative accuracy of the renormalized two-body formalism, we now compute the shear modulus of CFC states, C^t , as a function of filling factor. To this end, we utilize the following relation [38]: $C^t = \frac{1}{2}\nu^2 \frac{\partial^2}{\partial \nu^2} E^{2p\text{CFC}}$. It is important to note that this relation is derived under the assumption that only the two-body interaction is relevant, and is therefore consistent with our two-body formalism. Figure 3 shows C^t of various CFC states as a function of filling factor obtained by using $E_{\text{isol}}^{2p\text{CFC}}$ and $E_{\text{renorm}}^{2p\text{CFC}}$. While C^t obtained from the isolated two-body formalism is not to be trusted, it shows the relative importance of correlations from all surrounding CFs, which enhance C^t significantly. In particular, C^t in the renormalized two-body formalism shows a series of huge enhancements followed by discontinuous drops near $\nu = 1/(2p+1)$, which can be used as a distinctive signature for a phase transition between different CFC states.

Another important observable is the compressibility, whose inverse can be computed as follows [47]: $\kappa^{-1} =$

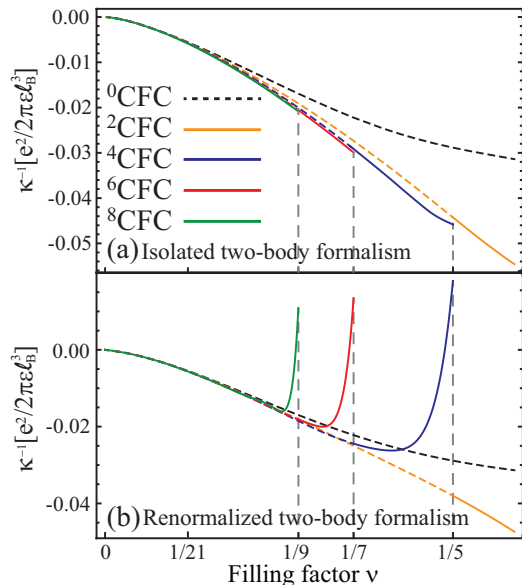


FIG. 4: (Color online) Inverse of the compressibility, κ^{-1} , of various CFC states as a function of filling factor, ν , obtained in (a) the isolated and (b) the renormalized two-body formalism. Similar to C^t , κ^{-1} of each ^{2p}CFC is valid only within the range of $1/(2p+3) < \nu \lesssim 1/(2p+1)$, where its curve is plotted in a solid line.

$\frac{1}{2\pi l_B^2} \nu^2 \frac{\partial^2}{\partial \nu^2} (\nu E^{2p\text{CFC}})$, where it is used that the electron density is related with the filling factor via $n = \nu/2\pi l_B^2$. Figure 4 shows κ^{-1} of various CFC states as a function of filling factor. At first sight, it may seem strange that the compressibility becomes negative in some regimes. This does not, however, mean an instability here since, by construction, we do not allow the positive background charge to relax. What we obtain above is the electronic part of the compressibility called the *proper* compressibility [48], which can be negative. In fact, the proper compressibility is directly measured in capacitive experiments [41–43] or by scanning single-electron transistor [44–46]. Compressibility has served as a powerful tool for detecting phase transitions between different fractional quantum Hall states as well as between differently spin polarized states at a given fraction [44–46]. Our calculations predict discontinuous changes in compressibility at the phase boundaries separating the different CFC phases, which can allow a determination of the phase diagram. Observation of such transitions inside the crystal phase will serve as direct evidence for the correlated CF character of WCs in the LLL, corroborating existing experimental indications of the CFC states [49, 50].

It is noteworthy that this is the first example where an accurate analytical treatment has become possible for a strongly correlated state in the LLL. It would be worth investigating if our method can be extended to the liquid states of CFs.

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