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Effect of Laughlin correlations on crystalline mean field solutions of the 2DEG in FQHE regime

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ABSTRACT

The energy per particle of many body wavefunctions that mix Laughlin liquid with crystalline correlations for periodic samples in the Haldane–Rezayi configuration is numerically evaluated for periodic samples. The Monte Carlo algorithm is employed and the wave functions are constructed in such a way that have the same zeroes as the periodic Laughlin states. Results with up to 16 particles show that these trial wavefunctions have lower energy than the periodic Laughlin states for finite samples even at $\nu = \frac{1}{3}$. Preliminary results for 36 particles suggest that this tendency could reach the thermodynamic limit. These results get relevance in view of the very recent experimental measures that indicate the presence of periodic structures in the 2DEG for extremely small temperatures and clean samples, inclusive at main FQHE filling fractions $\nu = \frac{1}{3}, \frac{2}{3}$.

Although the Fractional Quantum Hall Effect (FQHE) is described in its relevant aspects in terms of Jastrow-like many-body wave functions, a link between this variational approach and hamiltonian solutions is still desirable. The states introduced by Laughlin cleanly incorporate the tendency of particles to be as far away as possible from each other. On the other hand the Hartree–Fock states discussed in the literature (see [1] and the references therein) are approximate solutions of the Hamiltonian and may have valuable information not taken care of by the variational states. With this possibility in mind we have constructed a new type of trial wave function that incorporates a part of each approach as described below. Precisely in these days this construction gets relevance thanks to very recent experiments that had detected the presence of surprising periodic structures in the 2DEG for highly clean samples subject to extremely small temperatures [2]. Assuming that the proposed here wavefunctions maintain their properties of showing lower energies than the so called periodic Laughlin states (in the Haldane–Rezayi periodic scheme [3]) in the thermodynamic limit, they could have the opportunity of describing the detected periodic structures. Qualitatively, the energy dependence on the sample size obtained here suggests that the energy is lower in the limit of infinite size samples. However, this important conclusion needs for more extensive calculations for its full confirmation, that are expected to be considered elsewhere.

Analytic Hartree–Fock solutions in the lowest Landau level may be written down for filling fractions of the form $\nu = 1/q$. This unusual property was discovered after numerical results showed that there is a self-consistent charge density wave (CDW) solution to the Hartee–Fock (HF) equations that has a zero of order $q-1$ in each CDW plaquette. This property was then used to diagonalize the eigenvalue matrix. The resulting charge density corresponds to a lattice of holes, with percolating ridges that surround the zeroes. The form of the associated single particle wavefunctions suggests a way of constructing our new state incorporating both the Laughlin correlation in part, as well as the HF crystalline correlations (see [1]).

The appropriate framework to achieve this on the plane using numerical procedures is to impose periodic boundary conditions on the single particle states, as suggested by Haldane and Rezayi many years ago [3]. This is done in Ref. [4]. The main idea is to exploit the fact that the mean field Slater determinant in this picture can be written as the product of another determinantal function containing the whole dependence on the quantum numbers of the single particle HF states, times a factor whose zeroes are spatially fixed and periodic with the periodicity of the density. Therefore, the position of those zeroes has no dependence whatever on the set of quantum numbers of the filled mean field states, and has thus been factored out of the Slater determinant. Moreover, the number of zeroes of those kinematical factors as a function of any

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of the identical particle coordinates is just $(q-1)N_e$, where N_e is the number of electrons.

Let us begin by writing the explicit form of the counterparts of the Laughlin wavefunction in the Haldane–Rezayi scheme for implementing periodic boundary conditions

$$\Psi_L = \exp\Big(-\sum_{i=1,2,\ldots,N_e}\frac{y_i^2}{2r_o^2}\Big)\Big\{\vartheta_1\Big(\frac{\pi}{L}\big(Z^*-R^*\big)\Big|-\tau^*\Big)\Big\}^q \times \prod_{\substack{i<j\\ i,j=1,2,\ldots,N_e}}\Big\{\vartheta_1\Big(\frac{\pi}{L}\big(z_i^*-z_j^*\big)\Big|-\tau^*\Big)\Big\}^q,$$

where $z_j^* = x_j - iy_j$, $j=1,2,\ldots,N_e$ and $Z^* = X - iY$ are particles and center of mass complex coordinates, respectively. L is the cell size, $R^* = n_1a_1 + n_2a_2^*$ with n_1 and n_2 integers, $\tau^* = \exp(-2\pi i/6)$, and $a_1 = \sqrt{2\pi q/\sin(2\pi/6)}$, $a_2^* = a_1\tau$. The functions $\vartheta_1(u|\tau)$ are the odd elliptic theta functions and vanish as the first power in u as this variable goes to zero. We notice that as one particle approaches another, Ψ_L vanishes as a power q, so that altogether it includes $q(N_e-1)$ zeroes of this kind, plus q generated by the center of mass factor. We can thus replace the factors with spatially fixed zeroes in the HF solution, by a proper Laughlin factor to obtain the same short range behavior (a zero of order q) when any two particles approach each another. However, the presence now of the determinantal function keeps the crystalline information associated with the optimization of the mean field problem. Therefore, the proposed states have an a priori chance of lowering the energy per particle of the Laughlin states.

Then, in the Landau gauge $\mathbf{A} = -B(y,0,0)$, as it is proper of the Haldane–Rezayi scheme, the state ansatz being proposed here has the explicit form

$$\Psi = \Phi_L\big(z_1^*, z_2^*, \ldots, z_{N_e}^*\big)D\big[z_1^*, z_2^*, \ldots, z_{N_e}^*\big]\exp\Big(-\sum_{i=1,2,\ldots,N_e}\frac{y_i^2}{2r_o^2}\Big),$$

$$\Phi_L\big(z_1^*, z_2^*, \ldots, z_{N_e}^*\big) = \exp\big(-iQZ^*\big)\Big\{\vartheta_1\Big(\frac{\pi}{L}\big(Z^*-R^*\big)\Big|-\tau^*\Big)\Big\}^{q-1} \times \prod_{\substack{i<j\\ i,j=1,2,\ldots,N_e}}\Big\{\vartheta_1\Big(\frac{\pi}{L}\big(z_i^*-z_j^*\big)\Big|-\tau^*\Big)\Big\}^{q-1},$$

$$D\big(z_1^*, z_2^*, \ldots, z_{N_e}^*\big) = \mathrm{Det}\big[\chi_{\mathbf{k}_i}^{(0)}\big(z_k^*\big)\big], \tag{1}$$

where $Q = -\frac{\pi}{a}(q-1)$, $Z = \sum_{j=1}^{Ne} z_j$ and $r_0 = \sqrt{\hbar c/|eB|}$. The functions $\chi_{\mathbf{k}}^{(0)}$ have the form

$$\chi_{\mathbf{k}}^{(0)}(\mathbf{x}) = \exp\Big(i\varkappa z^* - \frac{y^2}{2r_o^2}\Big)\times\prod_R\vartheta_1\Big(\frac{\pi}{L}\big(z^*-R^*-C_{\mathbf{k}}\big)\Big|-\tau^*\Big).$$

Here $\varkappa = -\mathbf{k}\times\mathbf{a}_1/a_1$ and the argument $C_{\mathbf{k}}$ depending on the quantum number $\mathbf{k}$ is given by

$$C_{\mathbf{k}} = \frac{a}{2\pi}\big(-\mathbf{k}\times\mathbf{a}_2 - \mathbf{k}\times\mathbf{a}_1\tau^*\big) + \frac{qa\tau^*}{2}.$$

Our trial wave function Ψ is periodic, with a slanted periodicity region of equal sides length $L = Na_1$, and a slant angle of $2\pi/6$. The number of particles in the region is $N_e = N^2$. The momenta allowed by the periodic boundary conditions are

$$\mathbf{k} = \frac{n_1}{L}\mathbf{s}_1 + \frac{n_2}{L}\mathbf{s}_2,$$

where the reciprocal lattice unit vectors and the normal vector are defined by

Table 1
The results of the energy per particle for the counterparts of the Laughlin states in the Haldane–Rezayi periodic boundary conditions. The state for $N_e = 4$ was evaluated two times for different values of the Monte Carlo new configuration admission coefficient ξ in order to check the independence of its value. The calculations were done for $N_e = 4, 16$ particles.

$N_e = N^2$	ξ	ϵ
4	0.3	$-0.374476 \pm 0.0000697292$
4	0.25	$-0.374245 \pm 0.0000779082$
16	0.3	$-0.392032 \pm 0.0000880513$

Table 2
The results for the energy per particle for the trial state proposed in this work. The same Haldane–Rezayi periodic boundary conditions were employed. In this case the states for $N_e = 4, 16$ were evaluated two times each one for different values of ξ to check the independence of the result on this constant. The evaluations were done for $N_e = 4, 16$ and 36 particles in this case.

$N_e = N^2$	ξ	ϵ
4	0.2	$-0.414112 \pm 0.0000625317$
4	0.25	$-0.414191 \pm 0.0000457599$
16	0.25	-0.410156 ± 0.00006590
16	0.2	-0.410222 ± 0.00008659
36	0.25	$-0.410943 \pm 0.000486141$

$$\mathbf{s}_1 = -\frac{1}{qr_0^2}\mathbf{n}\times\mathbf{a}_2, \qquad \mathbf{s}_2 = \frac{1}{qr_0^2}\mathbf{n}\times\mathbf{a}_1,$$
$$\mathbf{n} = (0,0,1), \qquad \mathbf{a}_i\times\mathbf{s}_j = 2\pi\delta_{ij},$$

while the allowed values of n_1 and n_2 are

$$n_1 \in \Big\{-\frac{N}{2}, -\frac{N}{2}+1, \ldots, 0, \ldots, \frac{N}{2}-1\Big\},$$
$$n_2 \in \Big\{-\frac{N}{2}, -\frac{N}{2}+1, \ldots, 0, \ldots, \frac{N}{2}-1\Big\}.$$

The evaluations of the energy per particle of both states were done by employing the Monte Carlo method for samples having a number of particles N_e equal to 4 and 16 for the case of the Laughlin states. As for the trial wavefunctions investigated here the calculations were done for 4, 16 and 36 particles. The results are illustrated in Tables 1 and 2 and in Fig. 1. As mentioned before, the parameter ξ is the one defining the probability of admission of new configurations as usually is needed to do in the Monte Carlo algorithm. The margins of errors reported correspond to the maximum deviation from the mean value of a set of the last 60 percent of the evaluated energies in the Monte Carlo iterative process.

The expectation value of the many-particle Hamiltonian in the Laughlin state was evaluated using the Monte Carlo method for samples with $N_e = 4, 16$. For our trial wavefunctions calculations were done for 4, 16 and 36 particles. Results are shown in Tables 1 and 2. The parameter ξ defines the probability of admission of new configurations in the Monte Carlo algorithm. The errors reported in the third column correspond to the mean square of the fluctuations in the Monte Carlo output after convergence was assured. Our results are plotted in Fig. 1. The error bars are not resolved at the scale of the plot.

Note that a linear extrapolation to the thermodynamical limit $N->\infty$ of the Laughlin state energy reproduces former estimates of the energy of this state at $\nu = 1/3$. It is also clear that the energy per particle of each of the computed Laughlin values lies above that obtained for our trial wave function for any of the evaluated finite size samples. Moreover, the behavior of the energy of the latter for the largest number of particles evaluated, suggests that the energy per particle in the thermodynamic limit is lower than the one associated with the Laughlin state. In the contrary case, the extrapolation curve in the variable $1/N$ which join the

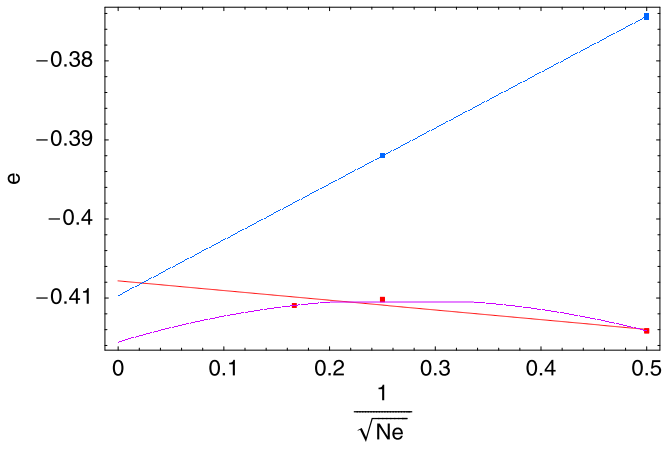

Fig. 1. Energy per particle as a function of the inverse square root of the number of particles $N = \sqrt{N_e}$. The picture shows that the introduction of correlations in the HF crystalline states made their energies lower than the ones shown by the versions of the Laughlin state in the Haldane–Rezayi periodic scheme. Note also that, if the behavior in the large N limit is confirmed by more extensive evaluations, the results will imply the existence of a ground state with a slightly lower energy than the Laughlin one for macroscopic samples. The curve joining the points of evaluated energies for the new trial state is a fitting of these three points to a quadratic polynomial in $1/\sqrt{N_e}$. The lower straight line with negative slope is simply a linear curve of $1/\sqrt{N_e}$ minimizing the mean square deviations from the three measured energies.

there three evaluated points of the energy $N = 2, 4$ and 6 should change its monotonic change of slope upon enlarging the value of N. However, being the number of Monte Carlo method iterations for the 36 particles state ($N = 6$) yet limited, this indication is not yet conclusive and further numerical evaluations will be done to give a better foundation to this conclusion. Its validity, clearly leads to the idea about that the recently detected periodic structures in extremely perfect 2DEG at very low temperatures, could be associated to the here proposed translation symmetry breaking states [2].

Let us now address a question that could arise in the readers in connection with the structure of the zeroes of the ansatz wavefunction (1). As it can be noticed, the position of the zeroes of the HF originated determinant (defined also in (1)) as a function of any of the electron coordinates, let say z_i^*, are precisely located at the rest of the electron coordinates z_j^*, for all values of j not coinciding with i. That is, the zeroes of the determinant as a function of any particular coordinate are coinciding with the ones associated to the Jastrow factors $\prod_{\substack{i<j \\ i,j=1,2,\ldots,N_e}} \{\vartheta_1(\frac{\pi}{L}(z_i^* - z_j^*)| - \tau^*)\}$, entering the definition of the Laughlin trial functions. Therefore, the above mentioned question might be posed as follows: Is not this described coincidence of a large set of zeroes, implying that the ansatz wavefunction should basically coincide with the Laughlin state for periodic boundary conditions (pbc), with the only freedom of a multiplicative center of mass wavefunction? However, in spite of the described shared common set of zeroes, it is possible to argue that the freedom within the *LLL* in functions having zeroes of order q for any electron coordinate z_i^* at the positions of the rest of all particles $z_j^* \neq z_i^*$, is in fact much larger than that one being spanned by a factor given by a center of mass coordinate wavefunction. The proof is simply following after considering the class of functions

$$\Psi_F = \prod_{k=1}^{Ne}\prod_{s=1}^{q}\left\{\vartheta_1\left(\frac{\pi}{L}\left(z_k^* - r_k^{s*}\right)\right| - \tau^*\right)\right\} \times \prod_{\substack{i<j \\ i,j=1,2,\ldots,N_e}} \left\{\vartheta_1\left(\frac{\pi}{L}\left(z_i^* - z_j^*\right)\right| - \tau^*\right)\right\}^q, \tag{2}$$

in which $r_k^{s*}, k = 1, \ldots, N_e$ and $s = 1, \ldots, q$ are the qN_e 2D zeroes within the principal region, of all the qN_e theta functions defining the first two products in the above formula. Note that q different positions of the zeroes for each coordinate, can be arbitrarily fixed. These wavefunctions all satisfy the periodic boundary conditions. This is indicated by the fact that they show a number of zeroes in the principal region, which coincides with the number of flux quanta piercing this region [3]. To see this property, note that there are qN_e theta functions entering in the first two products in (2), and only a finite set of q of them is associated to each one of the different electron coordinate of the N_e existing ones. Then, the fact that the specific theta functions ϑ_1 being employed in the definitions, show only one zero within the principal region, implies that the number of zeroes of (2) as a function of any of the particle coordinates is exactly qN_e. That is, as given by the sum of $q(N_e - 1)$ zeroes of the third product in (2) and the q zeroes shown by the corresponding product of q theta functions depending of the considered coordinate in the first two products appearing in (2).

The previous remark suggests an alternative proposal of ansatz wavefunctions which possibly can show a crystal symmetry. They will be defined as follows

$$\Psi_{tb}\left(z_1^*, \ldots, z_{N_e}^*\right) = \sum_P \left[\prod_k^{Ne}\prod_{s=1}^{q}\left\{\vartheta_1\left(\frac{\pi}{L}\left(z_{k^P}^* - R^*(k) - r_s\right)\right| - \tau^*\right)\right\}\right] \times \prod_{\substack{i<j \\ i,j=1,2,\ldots,N_e}} \left\{\vartheta_1\left(\frac{\pi}{L}\left(z_i^* - z_j^*\right)\right| - \tau^*\right)\right\}^q, \tag{3}$$

$$P\left(z_1^*, \ldots, z_{N_e}^*\right) = \left(z_{1^P}^*, \ldots, z_{N_e^P}^*\right),$$
$$P\left(1, 2, \ldots, N_e\right) = \left(1^P, 2^P, \ldots, N_e^P\right), \tag{4}$$

where P indicates the permutation of the coordinates as defined above. The function $R^*(k)$ is a bijective mapping of the integer particle indices $k = 1, \ldots, N_e$, to the lattice points generated by the unit cell vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, which also obey the condition of laying inside the first periodicity region. Note that the unit cell defined by $\mathbf{a}_1$ and $\mathbf{a}_2$ has q flux quanta passing through it, and thus, the number of lattice point being inside the periodicity region is just equal to N_e. The vectors r_s define an arbitrary set of q points inside each cell, devoted to set fixed relative positions within the lattice unit cells for the zeroes of the theta functions for each particular coordinate. The translation symmetric form of the definition suggests that in fact the proposed states could result to be equivalent, or contains as particular cases the ansatz states (1). These connections are expected to be investigated in coming extensions of the present work.

In ending we would like to underline that the present Letter consider a particular HF state showing one electron per its periodicity unit cell. For fillings of the form $1/q$ the HF solution produces a gap for all integers q. The experiment suggests, however, that even and odd q values are qualitatively different states. It has been shown in the past that if only half electron is captured by the unit crystalline cell this distinction is properly borne out [5]. Future work will extend to cover such states, and will be reported elsewhere. It should be underlined that similar searches to the one undertaken here, aiming to incorporate correlations in initial HF states, were before considered in the literature. In par-

ticular in Ref. [6,7], the investigation employed the disk geometry.

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