Bosonic quantum Hall states in single layer 2D optical lattices

Rukmani Bai,1,2 Soumik Bandyopadhyay,1,2 Sukla Pal,1 K. Suthar,1 and D. Angom1

1Physical Research Laboratory, Ahmedabad - 380009, Gujarat, India
2Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar - 382355, Gujarat, India

Quantum Hall (QH) states of two dimensional (2D) single layer optical lattices are examined using Bose-Hubbard model (BHM) in presence of artificial gauge field. We study the QH states of both the homogeneous and inhomogeneous systems. For the homogeneous case we use cluster Gutzwiller mean-field (CGMF) theory with cluster sizes ranging from $2 \times 2$ to $5 \times 5$. We, then, consider the inhomogeneous case, which is relevant to experimental realization. In this case, we use CGMF and exact diagonalization (ED). The ED studies are using lattice sizes ranging from $3 \times 3$ to $4 \times 12$. Our results show that the geometries of the QH states are sensitive to the magnetic flux $\alpha$ and cluster sizes. For homogeneous system, among various combinations of $1/5 \leq \alpha \leq 1/2$ and filling factor $\nu$, only the QH state of $\alpha = 1/4$ with $\nu = 1/2$, 1, 3/2 and 2 occur as ground states. For other combinations, the competing superfluid (SF) state is the ground state and QH state is metastable. For BHM with envelope potential, all the QH states observed in homogeneous system exist for box potentials, but none for the harmonic potential. The QH states also persist for very shallow Gaussian envelope potential. As a possible experimental signature we study the two-point correlations of the QH and SF states.

I. INTRODUCTION

The experimental realization of Bose Einstein condensates (BECs) of dilute atomic gases in optical lattices [1–4], and consequent developments [5, 6] have opened new frontiers to explore the physics of quantum many-body systems. This is due to the possibility of experimental control on the interatomic interactions, number of atoms, lattice geometry and choice of atomic species. In particular, bosons in optical lattices are near ideal realizations [7] of the Bose-Hubbard model (BHM) [8, 9]. The recent experimental implementations of artificial gauge field potential [10–16] in optical lattices have introduced an important parameter and made these systems excellent testing ground for QH physics [17]. Despite enormous progress in experimental and theoretical understanding of QH effect [18–21], a basic understanding of the fractional quantum Hall (FQH) effect [22] is still missing. The major difficulty arises from the strong correlations of electrons, but which is also the origin of FQH states. Although, the Laughlin ansatz [23] provides exact solutions for some FQH systems, but it is not yet observed in experiments. The strong magnetic field required to obtain FQH states is the major hurdle to observe these many-body states. Optical lattices, in this respect, have the advantage as various topological states, such as FQH states, are predicted to occur within the range of parameters achievable in experiments [24, 25].

In the BHM Hamiltonian the hopping and on-site interaction are the two competing terms. And both of these can be tuned by changing the depth of the lattice potential and employing Feshbach resonance [26, 27]. The hopping parameter $J$, which defines the strength of the hopping term in the BHM Hamiltonian, acquires a phase $J \rightarrow |J| \exp(i \Phi)$ in the presence of an artificial gauge potential [28] through the Peierls substitution [29, 30] and modifies the states of BHM. So, for an atom in the optical lattice there is a change of phase $\Phi = 2\pi \alpha$ when it hops around an unit cell or plaquette, where $\alpha$ is the flux quanta per plaquette. In theoretical studies, features of Laughlin states in low particle density limit has been reported [31] for $\nu = 1/2$ and $\alpha < \alpha_c = 0.4$. Here, $\nu$ is the filling factor, the number of particles per flux quanta and $\alpha_c$ is the critical value below which FQH states exist. For $\alpha > \alpha_c$ the equilibrium ground state properties start to change. And, the existence of a striped vortex lattice phase is reported in the neighbourhood of $\alpha = 1/2$ [32]. On the other hand, based on the results of Monte Carlo and exact diagonalization (ED), the existence of bosonic FQH states is predicted [33] in the vicinity of Mott plateaus for $\alpha = 2/3$. Similar results are reported in a recent work using the Chern-Simons theory [34] in combination with single site Gutzwiller mean-field (SGMF) theory. In another recent work [35], the incompressibility of the FQH states is employed to identify these states in computations using cluster Gutzwiller mean-field (CGMF) theory for $\alpha = 1/5$ at $\nu = 1/2$. On the other hand, using reciprocal cluster mean-field (RCMF) analysis Hügel et al. [36] predicted a competing FQH state as a metastable state for $\alpha = 1/4$. In this work, we report FQH states at distinct $\nu$s for low and high flux. For example, when $\alpha = 1/5$ we obtain QH states at $\nu = n/2$, where $n = 1, 2, \ldots, 9$ and for $\alpha = 1/2$ at $\nu = 1/2, 1,$ and $3/2$. In particular, we discuss the QH states for $\alpha = 1/5, 1/4$ and $1/2$ in the hard-core boson limit. We also obtain QH states for $\alpha = 1/3$ case, however, we have not provided the details as the general trend is similar to $\alpha = 1/5$.

Motivated by the recent theoretical investigations and experimental progress, we address a basic gap in our current understanding. And, that is the occurrence of QH states in optical lattices with an envelope potential. This key issue is addressed in this work. For our studies we use SGMF [37–39] and CGMF [40–44] theories, and ED. Our results, for the case of homogeneous optical lattices, agree well with the previous theoretical observations. After establishing this and demonstrating that getting the geometry of QH states requires larger cluster sizes in CGMF, we provide an answer to the question: what is the nature of the QH states in optical lattices with an envelope potential?
II. THEORETICAL METHODS

We consider bosonic atoms at zero temperature confined in a two-dimensional (2D) square optical lattice with an envelope potential in presence of synthetic magnetic field [14–16, 45]. In the Landau gauge, the system is well described by the BHM [7, 24, 25, 32, 45] with Peierls substitution in the nearest-neighbour (NN) hopping [29, 30, 46], and the Hamiltonian is

\[ \hat{H} = -\sum_{p,q} \left[ \left( J_x e^{i2\pi\alpha_q} \hat{b}_{p+1,q}^\dagger \hat{b}_{p,q} + \text{H.c.} \right) + \left( J_y \hat{b}_{p,q+1}^\dagger \hat{b}_{p,q} + \text{H.c.} \right) \right] + \sum_{p,q} \left[ \frac{U}{2} \hat{n}_{p,q}(\hat{n}_{p,q} - 1) - (\mu - \varepsilon_{p,q})\hat{n}_{p,q} \right]. \]  

(1)

where \( p \) (\( q \)) is the lattice site index along \( x \) (\( y \)) direction, \( \hat{b}_{p,q} \) (\( \hat{b}_{p,q}^\dagger \)) is the bosonic annihilation (creation) operator, and \( \hat{n}_{p,q} \) is the number operator. The parameter, \( J_x \) (\( J_y \)) is the complex hopping strength between two NN sites along \( x \) (\( y \)) direction, \( U \) is the on-site interaction strength. Here, \( \mu \) is the chemical potential and \( \varepsilon_{p,q} \) is the energy offset of the envelope potential.

The envelope or confining potential, in the case of harmonic potential, modifies \( \mu \) by the energy offset \( \varepsilon_{p,q} = \Omega(p^2 + q^2) \), where \( \Omega \) is the strength of the harmonic confining potential. The phase \( 2\pi\alpha \) in \( J_x \) arises from the synthetic magnetic field and \( 0 \leq \alpha \leq 1/2 \). It is well established that for \( \alpha = 0 \) the phase diagram of BHM admits two phases, Mott insulator (MI) and superfluid (SF) phase [3, 7, 8]. The strong on-site interaction limit \( (J/U \ll 1) \) corresponds to the MI phase, whereas the opposite limit \( (J/U \gg 1) \) corresponds to the SF phase. The phase diagram in the \( \mu - J \) plane consists of Mott lobes with increasing commensurate integer filling.

And, it has been shown in previous studies that MI lobes are enlarged for \( \alpha \neq 0 \) [47].

A. Gutzwiller mean-field theory

To obtain the eigenstates of BHM, we use the mean-field approximation [38]. For the mean-field Hamiltonian, the annihilation (creation) operators in Eq. (1) are decomposed as

\[ \hat{b}_{p,q} = \phi_{p,q} + \Delta \hat{b}_{p,q}, \]  

(2a)

\[ \hat{b}_{p,q}^\dagger = \phi^*_{p,q} + \Delta \hat{b}_{p,q}^\dagger, \]  

(2b)

where \( \phi_{p,q} = \langle \hat{b}_{p,q} \rangle \) is the SF order parameter, and \( \phi^*_{p,q} = \langle \hat{b}_{p,q}^\dagger \rangle \). Using these definitions in Eq. (1) and neglecting the second order term in fluctuations like \( \Delta \hat{b}_{p+1,q}^\dagger \Delta \hat{b}_{p,q} \), we obtain the mean-field Hamiltonian of the BHM as

\[ \hat{H}^{MF} = -\sum_{p,q} \left[ \left( J_x e^{i2\pi\alpha_q} \phi_{p+1,q} + \phi^*_{p,q} \right) \hat{b}_{p,q}^\dagger \hat{b}_{p,q} + \phi_{p,q}^* \hat{b}_{p+1,q}^\dagger \hat{b}_{p,q} + \phi_{p,q} \hat{b}_{p,q}^\dagger \hat{b}_{p,q}^\dagger + \text{H.c.} \right] \]

\[ + \sum_{p,q} \left[ \frac{U}{2} \hat{n}_{p,q}(\hat{n}_{p,q} - 1) - (\mu - \varepsilon_{p,q})\hat{n}_{p,q} \right]. \]  

(3)

The order parameter \( \phi_{p,q} \) is zero for the MI phase and finite for the SF phase. The Hamiltonian in Eq. (3) can be considered as the sum of the single-site Hamiltonian

\[ \hat{h}_{p,q} = -\left[ J_x e^{i2\pi\alpha_q} \left( \phi^*_{p+1,q} \hat{b}_{p,q}^\dagger - \phi_{p,q} \hat{b}_{p,q} \right) + \phi_{p,q}^* \hat{b}_{p,q}^\dagger \hat{b}_{p,q} + \phi_{p,q} \hat{b}_{p,q}^\dagger \hat{b}_{p,q}^\dagger + \text{H.c.} \right] \]

\[ + \sum_{p,q} \left[ \frac{U}{2} \hat{n}_{p,q}(\hat{n}_{p,q} - 1) - (\mu - \varepsilon_{p,q})\hat{n}_{p,q} \right]. \]

(4)

We can, therefore, diagonalize the Hamiltonian for each site separately. To compute the ground state of the system, we use the site dependent Gutzwiller ansatz. That is, the ground state of the system is the direct product of the ground states of all the sites,

\[ |\Psi_{GW}\rangle = \prod_{p,q} |\psi_{p,q}\rangle = \prod_{p,q} \sum_{n=0}^{N_{b}} c_{n}^{(p,q)} |n\rangle_{p,q}, \]  

(5)

where \( N_{b} \) is the highest occupation number basis state, \( c_{n}^{(p,q)} \) are the complex coefficients of the ground state \( |\psi_{p,q}\rangle \) at the site \( (p,q) \) with the normalization condition \( \sum_{n} |c_{n}^{(p,q)}|^2 = 1 \). Then, the SF order parameter at the lattice site \( (p,q) \) is

\[ \phi_{p,q} = \langle \Psi_{GW} | \hat{b}_{p,q}^\dagger \Psi_{GW} \rangle = \sum_{n=0}^{N_{b}} \sqrt{n} c_{n+1}^{(p,q)^*} c_{n}^{(p,q)}. \]  

(6)

Based on the definition of \( |\Psi_{GW}\rangle \) in Eq. (5), the MI state with density or occupancy \( \rho = m \) is

\[ |\Psi_{GW\text{MI}}\rangle = \prod_{p,q} c_{m}^{(p,q)} |m\rangle_{p,q}, \]  

(7)

with the condition \( |c_{m}^{(p,q)}|^2 = 1 \). Considering the above expression, it is evident that \( \phi_{p,q} \) is zero in the MI phase of the system. But \( \phi_{p,q} \) is finite for the SF phase as more than one occupation number state contribute to \( |\psi_{p,q}\rangle \). As the inter-site coupling is through \( \phi_{p,q} \), and it cannot describe strongly correlated FQH states. For this reason, previous works have relied on CGMF [35] and RCMF [36] to obtain FQH states in BHM. In the present work, to obtain ground state, the mean-field Hamiltonian is diagonalized for each lattice site with \( N_{b} = 10 \) using initial guess of \( \phi_{p,q} \). After diagonalization, the ground state is retained as the state \( |\psi_{p,q}\rangle \) of the site in \( |\Psi_{GW}\rangle \). In addition, using \( |\psi_{p,q}\rangle \) a new \( \phi_{p,q} \) is computed and this cycle is continued till convergence.
The Hamiltonian for a cluster can be written as
\[ \hat{H}_C = -\sum_{p,q \in C} \left[ \left( e^{i\pi \alpha q} J_x \hat{b}_p^\dagger \hat{b}_{p+q} + H.c. \right) + \left( J_y \hat{b}_p^\dagger \hat{b}_{p+1,q} + H.c. \right) \right. \\
\left. - \sum_{p,q \in \delta C} \left[ \left( e^{i\pi \alpha q} J_x \hat{b}_p^\dagger \hat{b}_{p+q} + H.c. \right) + \left( J_y \hat{b}_p^\dagger \hat{b}_{p+1,q} + H.c. \right) \right. \\
\left. + \left( \frac{U}{2} \hat{n}_{p,q} (\hat{n}_{p,q} - 1) - (\mu - \varepsilon_{p,q}) \hat{n}_{p,q} \right) \right] , \]
where the prime in the summation of the first term is to indicate that \((p + 1, q), (p, q + 1) \notin C\) and \(\delta C\) represents the lattice sites at the boundary of the cluster. The order parameter \(\phi^*_{p+1,q} = \langle \hat{b}_{p+1,q}^\dagger \rangle\) with \((p + 1, q) \notin C\) defines the order parameter at the boundary of the neighbouring cluster and is required to describe the inter-cluster hopping along the \(x\) direction. Similarly, \(\phi^*_{p,q+1} = \langle \hat{b}_{p,q+1}^\dagger \rangle\) with \((p, q + 1) \notin C\). Schematically, the clusters are conveniently represented in terms of cells. In Fig. 2 the cells of a \(2 \times 2\) cluster and neighbouring clusters are highlighted.

To obtain the ground state with CGMF, we diagonalize the cluster Hamiltonian and the ground state of the cluster in the Fock basis is
\[ |\Psi_c \rangle = \sum_{n_{0 \ldots \ell} \ldots n_{m'}} C_{n_{0 \ldots \ell} \ldots n_{m'}} |n_{0 \ldots \ell} \ldots n_{m'} \rangle , \]
where \(n_{m'} = (M \times N) - 1\) and \(n_i\) is the index of the occupation number state of \(i\)th lattice site within the cluster, and \(C_{n_{0 \ldots \ell} \ldots n_{m'}}\) is the amplitude of the cluster Fock state \(|n_{0 \ldots \ell} \ldots n_{m'} \rangle\). The above definition can be written in a more compact form using the index quantum number \(\ell \equiv \{n_{0 \ldots \ell} \ldots n_{m'}\}\) as
\[ |\Psi_c \rangle = \sum_{\ell} C_{\ell} |\Phi_c \rangle_{\ell} , \]
where \(|\Phi_c \rangle_{\ell}\) represents the cluster basis state \(|n_{0 \ldots \ell} \ldots n_{m'}\rangle\).

As mentioned in the previous works [34, 35], the convergence is very sensitive to the initial conditions, and to accelerate convergence we use the method of successive over-relaxation [48].
FIG. 3. The $M \times 1$ row of a cluster with occupation number $n_0, n_1, \ldots, n_{M-1}$. Each square box represents a lattice site and each of $n_i$ corresponds to $i$th lattice site in that row. Here, $n_i$ runs from 0 to $N_b - 1$ for each lattice site.

C. Exact Diagonalization Method

For an $M \times N$ lattice the computations with ED method are done with the BH Hamiltonian

$$\hat{H} = - \sum_{0 \leq p < M, 0 \leq q < N} \left( J_x e^{i2\pi\alpha q} \hat{b}^\dagger_{p+1,q} \hat{b}_{p,q} + J_y \hat{b}^\dagger_{p,q+1} \hat{b}_{p,q} \right) + \text{H.c.} + \sum_{0 \leq p < M, 0 \leq q < N} \frac{U}{2} \hat{n}_{p,q} (\hat{n}_{p,q} - 1). \quad (13)$$

Here, $\mu$ is not required as, unlike the mean field theories, the number of atoms is fixed and the computations are in the corresponding Hilbert space. The Hilbert space is spanned by the states $|\Psi_c\rangle$, which like in CGMF can be considered as states of one $M \times N$ cluster, and the ground state is obtained by diagonalizing the Hamiltonian matrix. For compact notation, we consider each $|\Psi_c\rangle$ is a direct product of $N$ row states, and each row state is represented as

$$|\phi\rangle_m = \prod_{i=0}^{M-1} |n_i\rangle,$$

where, $0 \leq i \leq M - 1$ are lattice sites along $x$ direction, $|n_i\rangle$ is the occupation number state at $i$th lattice site and $m \equiv \{n_0, n_1, \ldots, n_{M-1}\}$ is an index quantum number of the row state. The schematic representation of a row state is shown in Fig. (3). Thus, one of the cluster states can be written as

$$|\Phi_c\rangle_\ell = \prod_{j=0}^{N-1} |\phi^j\rangle_{m,j} = \prod_{j=0}^{N-1} \prod_{i=0}^{M-1} |n^j_i\rangle,$$

where, $0 \leq j \leq N - 1$ represent row of the cluster as shown in Fig. (4), and we have introduced cluster state index quantum number $\ell \equiv \{n^0_0, n^1_0, \ldots, n^{N-1}_0, n^0_1, n^1_1, \ldots, n^{N-1}_1, \ldots, n^0_{M-1}, n^1_{M-1}, \ldots, n^{N-1}_{M-1}\}$, which is essentially equivalent to writing $\ell \equiv \{m^0, m^1, \ldots, m^{N-1}\}$. In short, as shown in Fig. (4) there is a hierarchy of states, the single site occupation number states $|n^j_i\rangle$, the row states $|\phi^j\rangle_m$ and cluster states $|\Phi_c\rangle_\ell$.

Now to construct the Hilbert space, consider the total number of atoms to be $N_a$, and for the present work as we consider low density $N_a \ll M \times N$. We can, therefore, consider the occupation number state at each lattice site to vary from say $|0\rangle$ to $|1\rangle$, and consider the total number of atoms in the row states $|\phi^j\rangle_m$ as $0 \leq \sum_i |n^j_i| \leq \min(M, N_a)$. However, the cluster states $|\Phi_c\rangle_\ell$ are direct product states of $|\phi^j\rangle_m$ such that the total number of atoms in $|\Phi_c\rangle_\ell$ is $N_a$, that is

$$\sum_{i=0}^{M-1} \sum_{j=0}^{N-1} n^j_i = N_a. \quad (16)$$

After diagonalizing the Hamiltonian in Eq. (13) (for details see the appendix), we can get the ground state as

$$|\Psi_c\rangle = \sum_\ell C_\ell |\Phi_c\rangle_\ell,$$

where $C_\ell$ is the coefficient of the cluster state and normalization of the state is ensured through the condition $\sum_\ell |C_\ell|^2 = 1$. The normalization, however, is guaranteed as the Hamiltonian is Hermitian. As explained in appendix, the general features of the ED method described here can be extended to the CGMF theory to compactify the Fock space used in the computations.

III. RESULTS AND DISCUSSIONS

To examine the effect of additional correlation in the CGMF compared to SGMF we compute the phase diagram using the two methods in presence of artificial gauge field. For the SGMF we choose the basis set of each lattice site as $\{|0\rangle_{p,q}, |1\rangle_{p,q}, \ldots, |9\rangle_{p,q}\}$. And, for the CGMF computations we consider a cluster basis consisting of single site occupation number states $\{|0\rangle, |1\rangle\}$. As an example, the $\rho = 1$ Mott lobe obtained from SGMF and CGMF with $3 \times 2$ clusters for $\alpha = 1/3$ is shown in Fig. 5.
Based on the figure, the Mott lobe obtained from the CGMF is larger than the SGMF. This indicates that the CGMF provides a better description of the strongly correlated state like the MI phase better. The other important observation from the figure is that, the artificial gauge field enhances the Mott lobe. This is expected as the synthetic magnetic field induced cyclotron motion suppress the itinerant character of atoms in the SF phase, and supports MI phase due to the localization effect [49]. Our phase diagram from the SGMF theory is consistent with the results of Ref. [34].

The CGMF computations are done with clusters which are integer multiple of the magnetic unit cell. As we consider a system where the flux $\Phi$ is staggered along $y$-axis, for $\alpha = 1/N$, a $1 \times N$ cluster forms a magnetic unit cell. We, however, find that except for a $\pi/2$ rotation the results are identical to $N \times 1$ cluster. This is due to the coupling of motion along $x$ and $y$ through the interparticle interaction. The states obtained are classified based on the compressibility $\kappa = \partial \rho / \partial \mu$, where the density $\rho = \sum_j |\psi_j|^2 n_j |\psi_j|^2 / (K \times L)$. For the QH states $\kappa = 0$ or it is incompressible, and $\kappa > 0$ for the SF states. As a result, QH states manifest as plateaus in $\rho(\mu)$ for different $\nu$ and it is linear for the SF phase. Thus, in Fig. 6 the horizontal lines indicating constant $\rho$ define the existence of QH states. Here, for simplicity and to be consistent with the experimental realizations we consider isotropic hopping, $J_x = J_y = J$, and repulsive on-site interaction, $U > 0$.

A. Homogeneous system

Based on our results, only the QH states for $\alpha = 1/4$ and $\nu = 1/2$, $1/3/2$ and $2$ are ground states when $J/U \approx 0.01$, and the competing SF state is metastable. For the mentioned values the QH state is the ground state over a small range of $\mu$ centered around $-0.019U$, $-0.014U$, $-0.007U$ and $0.000U$, respectively. For the other combination of $\alpha$ and $\nu$ the SF and QH states are ground and metastable states, respectively. In general, for different $\alpha$, the energy difference between the SF and QH states $\Delta E \approx 10^{-3}U$. For the parameters of experimental interest $U/h = 130$ Hz [50] and we get $\Delta E \approx 10^{-2}$K. This implies stringent bounds on the thermal excitations during the state preparation to obtain QH states. One feature of the CGMF results which distinguishes the QH states from the SF states is the energy. For the QH state the energy decreases with increasing cluster size. For example the QH state of $\alpha = 1/4$ with $\nu = 1/2$ and $\mu = -0.02U$ has energy $-0.0031U$ and $-0.0046U$ with $2 \times 4$ and $4 \times 4$ clusters, respectively. Whereas for the SF state, the energy remains almost unchanged as it is $-0.0042U$ and $-0.0045U$, respectively. Thus, the QH state emerges as the ground state with the $4 \times 4$ cluster. Here, the key point is not the values of the energies per se, but the importance of having better correlation effects to obtain QH states. These trends arise from the better description of the hopping term with larger cluster size. Besides $\alpha = 1/4$, the other values of $\alpha$ we have studied in detail are $1/5$ and $1/2$. Results for each of the $\alpha$ considered are described.

I. $\alpha = 1/5$

For the hard-core boson limit, where $\rho < 1$, with $\alpha = 1/5$, we obtain QH states for $\nu = n/2$, where $n = 1, 2, \ldots, 9$ with $2 \times 5$ cluster. The case of $\nu = 1/2$ was reported by Natu et al. [35], and as shown in Fig. 7 our results are consistent. Among the new FQH states we have identified $\nu = 3/2, 7/2, and 9/2$ are stripe phase whereas it is homogeneous for $\nu = 5/2$. In addition, we obtain stripe phase integer QH (IQH) states for
The other distinguishing feature of $\nu = 2$ and $5/2$ is that the competing SF states have zigzag order in $\rho$ and $\phi$. On increasing the cluster size to $3 \times 5$ the QH states with stripe geometry are transformed to checkerboard, and the density contrast is reduced on increasing the cluster size to $4 \times 5$. We also obtain the same QH states but rotated by $\pi/2$ when the cluster sizes are $5 \times 2$, $5 \times 3$ and $5 \times 4$. For example with $5 \times 2$ cluster the stripe order is horizontal while it is vertical for $2 \times 5$ cluster. Considering this property of QH states, and noting that $1 \times 5$ is the magnetic unit cell for $\alpha = 1/5$, an accurate description of the FQH state is possible with $5 \times 5$ cluster. With this cluster size the operator part of the hopping term in Eq. (1) is exact along $x$ and $y$ axis within the cluster symmetrically. For example, with $2 \times 5$ cluster, hopping along $x$ axis has contribution through mean-field after $2a$ while it is $5a$ for $5 \times 5$ cluster, where $a$ is lattice constant.

2. $\alpha = 1/4$

For the case of $\alpha = 1/4$, we obtain QH states for $\nu = n/2$, where $n = 1, 2, \ldots, 7$, with $2 \times 4$ and $4 \times 4$ clusters. The FQH states for $\nu = 1/2, 3/2, 5/2$ have stripe order with $2 \times 4$ cluster, however, like in the case of $\alpha = 1/5$ is transformed into checkerboard order with $4 \times 4$ cluster. That is, the geometry depends on the cluster size. Furthermore, as we increase the cluster size to $4 \times 8$ the FQH state with $\nu = 1/2$ filling remain qualitatively unchanged. For the IQH states the $\nu = 1$ and $3$ have stripe order with $2 \times 4$ cluster and checkerboard with $4 \times 4$ cluster. But, the IQH state corresponding to $\nu = 2$ has homogeneous density order. It must be mentioned that the thermodynamic limit, due to the coupling of neighbouring clusters through $\phi$, does not apply to CGMF description of QH states where $\phi = 0$. This limits the applicability of the theory to finite size systems relevant to experimental realizations in optical lattices. On the other hand for the competing SF state a large lattice size, due to the finite $\phi$, corresponds to the thermodynamic limit.

3. $\alpha = 1/2$

For the high flux $\alpha = 1/2$, we again consider $2 \times 4$ and $4 \times 4$ clusters in the CGMF computations. It must be emphasized that $\alpha = 1/2$ is relevant to the recent experimental realizations [15, 16]. For this value of $\alpha$, we obtain the QH states for $\nu = 1/2, 1$, and $3/2$ from both the clusters. Like in $\alpha = 1/5$ and $1/4$ cases, the $\nu = 1/2$ and $3/2$ FQH and SF states are stripe and homogeneous phases, respectively, with $2 \times 4$ cluster. The structure of the FQH state is transformed into checkerboard with $4 \times 4$ cluster. This transformation is visible from the variation in $\rho$ for the case of $\nu = 1/2$ as shown in Fig. 8. For $\nu = 1$ the IQH and SF states are homogeneous for both the cluster sizes. An important observation is, the homogeneous QH state is generic to $\rho = 0.5$ for the values of $\alpha$ considered in the present work.

B. Inhomogeneous system

The simplest modification to the homogeneous system for comparison with experimental realizations is to impose hard-wall boundary conditions. This corresponds to the 2D optical lattice realization similar to the case of homogeneous BEC in a box potential [51]. With the hard-wall boundary we recover the QH states for all $\alpha$ as described earlier, and energies remain unchanged. The competing SF states, on the other hand, have higher energies with hard-wall boundary. In the present work the largest cluster size in the CGMF computations required to encapsulate one magnetic unit cell along $y$-axis and maintain symmetry in the exact description of hopping term is $5 \times 5$ for $\alpha = 1/5$. For this reason, we focus on the properties of the QH states of $\alpha = 1/5$. The other QH states are qualitatively similar, but computationally less demanding. It is also to be
emphasized that the results of single cluster with hard-wall boundary is equivalent to ED. Because with hard wall boundary, we do not employ the periodic boundary condition, thus the mean field part vanishes and Hamiltonian becomes exact.

The IQH state for $\nu = 1$ with different cluster sizes are shown in Fig. 9, which has stripe geometry. In the homogeneous case, the stripe geometry is transformed into checkerboard geometry with $3 \times 5$ cluster. However, the most important observation is that $\rho(x, y)$ obtained from $3 \times 5$ cluster, although checkerboard in structure, is very different from that of $3 \times 5$ and $4 \times 5$, which are shown in Fig. 10. An observable property to identify the QH states is the two-point correlation function $\langle \hat{b}_x^\dagger(y)\hat{b}_0(y) \rangle$, where the expectation is computed with respect to $|\psi_c\rangle$, and the results from the $5 \times 5$ cluster are as shown in Fig. 11(a). The two-point correlation function is closely related to another important property, the one body density matrix (OBDM) \cite{52, 53}

$$\rho_{k,l} = \langle \psi_c | \hat{b}_{k}^\dagger \hat{b}_{l} | \psi_c \rangle,$$

where $k \equiv (x, y)$ and $l \equiv (x', y')$ are lattice indices. From the OBDM one can compute the condensate fraction based on Penrose-Onsager criterion \cite{54} and von Neumann entropy \cite{55–57}. These measures are particularly relevant to ED method and are described while discussing the ED results. The correlation function, as recently proposed, could be measured with quantum probes \cite{58, 59}. As reported in a recent work \cite{60}, it can be seen from the figure that $\langle \hat{b}_x^\dagger(y)\hat{b}_0(y) \rangle$ decays as inverse power law at the edge. However, in the bulk, it is gapped, it initially shows exponential decay $\langle \hat{b}_x^\dagger(y)\hat{b}_0(y) \rangle \propto e^{-x/\xi}$ but it is power law when $x > K/2$ or on reaching the opposite edge. Here, $\xi$ is the correlation length of the system and as mentioned earlier, $K$ is the size of the cluster along $x$. For the SF state with $5 \times 3$ cluster, as seen from Fig. 11(b), the correlation through the bulk does not show any nonmonotonicity. Here, we have considered $5 \times 3$ cluster as the correlation in the bulk is not sensitive to the size of the cluster.

The other envelope potential which is of experimental relevance is the harmonic oscillator potential. Then, the energy offset $\varepsilon_j = \Omega j^2 = \Omega(p^2 + q^2)$, $\Omega$ is the strength of the potential. To encapsulate the envelope potential, we consider a larger lattice size ranging from 40 $\times$ 40 to 80 $\times$ 80. We, however, find that the QH states are absent. This is due to the nature of $\partial \varepsilon_j / \partial j$, it monotonically increases and does not favour incompressible phase like QH state. One possible modification is that the beam waist $w$ of the laser beam generating the envelope potential is large. So that, the effective envelope potential is still a Gaussian $V_{C2} = U_0 e^{-(a^2+b^2)/w}$. Here, the amplitude of the Gaussian potential $U_0$ is proportional to the intensity of the laser beam. With this potential, $\partial \varepsilon_j / \partial j$ also decays exponentially and we find that the QH states exist for $U_0 \lesssim 10^{-3} U$. At higher values of $U_0$ only the SF state is obtained from the CGMF computations.

FIG. 9. Density distribution of the IQH state for $\alpha = 1/5$ and $\nu = 1$ with hard-wall boundary. The average density of atoms in this state is $\rho = 0.2$. (a) The IQH state has stripe geometry in the CGMF results with $2 \times 5$ clusters. (b) It is, however, transformed to checkerboard geometry when $3 \times 5$ clusters are considered in the CGMF computations.

FIG. 10. The variations in $\rho$ for IQH state of $\alpha = 1/5$ and $\nu = 1$ for a single cluster of different sizes. (a) The result from $3 \times 5$ cluster has checkerboard pattern, and is the unit cell of the large lattice shown in Fig. 9. (b) $4 \times 5$ cluster has less variations in $\rho$ compared to $3 \times 5$. (c) $5 \times 5$ cluster shows a rich variation in $\rho$ and unlike in (a) and (b) the central lattice site has maxima in density.

FIG. 11. Two-point correlation function for low flux $\alpha = 1/5$ with the $5 \times 5$ and $5 \times 3$ clusters for the QH and SF states, respectively. The correlation is calculated along the $x$ direction for the single cluster. Here $y = 0$ and $1$ represent the edge and bulk states, respectively. (a) As a characteristic feature of QH state, the correlation function of the $\nu = 1$ IQH state decays nonmonotonically in the bulk, and there is no difference between the hard-wall and periodic boundary conditions. (b) For the corresponding SF state there is no trend in the bulk correlation function with hard-wall boundary (solid green line with down triangle symbol), but it decays monotonically at the edge (solid brown line with circle symbol). With periodic boundary condition (dashed lines), the range of values change, and both the bulk and edge exhibit monotonic decay in correlation.
C. ED results

With the ED computations [52, 53], we focus our attention on the $\alpha = 1/4$, which have QH states as ground state. For this we, in particular, consider $\nu = 1/2$ FQH state with cluster sizes $4 \times 4$, $4 \times 8$, and $4 \times 12$. Here, as alluded earlier, we distinguish the QH states and SF states based on the Penrose-Onsager criterion [54] and von Neumann entropy [55–57]. For this, we compute OBDM in Eq. (18), and then digonalize it. Following the Penrose-Onsager criterion, the state is SF if $p_m = \lambda_{OBDM}^m / N \approx 1$, where $\lambda_{OBDM}^m$ is the largest eigenvalue of the OBDM, and $N$ is the total number of atoms. In contrast, for the QH states $p_m < 1$. Our results are in agreement with this, for example, with $4 \times 4$ cluster, the values of $p_m$ are 0.56 and 0.89 for the FQH and SF states, respectively. Once the OBDM is diagonalized, the von Neumann entropy is defined as

$$ S = - \sum_i p_i \ln(p_i), \quad (19) $$

where $p_i = \lambda_i^{OBDM} / N$ and $M$ is dimension of the OBDM. As the von Neumann entropy is a measure of entanglement, it is higher for the more correlated states like QH states compared to the SF states. For the states considered the values of $S$ are 1.0 and 0.53 for the FQH and SF states, respectively. These values indicate that the FQH state, as expected, is more entangled than the SF state. When the cluster size is increased to $4 \times 8$ the value of $p_m$ is modified to 0.26 and 0.80 for the FQH and SF states, respectively. And, the corresponding values of $S$ are 1.84 and 0.95, respectively. We also obtain similar results for the other QH and SF states, for example, $p_m$ is 0.33 and 0.75 for the QH and SF states respectively with $5 \times 5$ cluster for $\alpha = 1/5, \nu = 1$. The corresponding value of $S$ is 1.89 and 1.20 respectively. It is to be mentioned here that the QH and SF states obtained from the ED method have the same features, $\rho$ and $\phi$, as in CGMF results.

IV. CONCLUSIONS

Based on the results of our studies with CGMF and ED, the $\alpha = 1/4$ with $\nu = 1/2, 1, 3/2$ and 2 are the QH states which occur as ground state of the BHM with synthetic magnetic field, and these states exist within a narrow range of $\mu$. For other combinations of $\alpha$ and $\nu$, the SF state is the ground state and the QH state exist as a metastable state. The experimental observation of a pure QH state needs tight control on the thermal excitations as the two competing states, QH and SF states, are nearly degenerate. The separation is only $\approx 10^{-2}\hbar K$. Furthermore, the QH state is sensitive to the nature of the envelope potential of the optical lattice. The QH states exist for very shallow Gaussian envelope potentials but cease to exist when the envelope potential is harmonic. The case of a box potential is the most promising experimentally realizable envelope potential to observe a pure QH state of BHM with synthetic magnetic field.

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APPENDIX

To illustrate the form of the Hamiltonian in CGMF, consider the BHM Hamiltonian for a $2 \times 2$ cluster located at the bottom right of the lattice in Fig. 1 is

$$ \hat{h}_c = \hat{h}_{00} + \hat{h}_{10} + \hat{h}_{01} + \hat{h}_{11}, $$

where $\hat{h}_{pq}$ is the single-site Hamiltonian at the $(p, q)$ lattice sites within the cluster. In general, if the lattice considered is $K \times L$, then the lattice sites are labeled along $x$ ($y$) axis as $0, 1, \ldots, K - 1 (0, 1, \ldots, L - 1)$. The expression of the single-site Hamiltonians are

$$ \hat{h}_{00} = - \left( J_x \hat{b}^\dagger_{1,0} \hat{b}_{0,0} + H.c. \right) - \left( J_y \hat{b}^\dagger_{0,1} \hat{b}_{0,0} + H.c. \right) - \left[ J_x \left( \hat{b}_{0,0}^\dagger \phi_{K-1,0} - \phi_{0,0}^* \phi_{K-1,0} \right) + H.c. \right] $$

$$ - \left[ J_y \left( \hat{b}_{0,0}^\dagger \phi_{0,L-1} - \phi_{0,0}^* \phi_{0,L-1} \right) + H.c. \right] + \frac{U}{2} \hat{n}_{0,0}(\hat{n}_{0,0} - 1) - \mu \hat{n}_{0,0}, \quad (20) $$

$$ \hat{h}_{10} = - \left( J_y \hat{b}^\dagger_{1,1} \hat{b}_{1,0} + H.c. \right) - \left[ J_x \left( \phi_{2,0}^* \hat{b}_{1,0} - \phi_{2,0} \phi_{1,0} \right) + H.c. \right] - \left[ J_y \left( \hat{b}_{1,0}^\dagger \phi_{1,L-1} - \phi_{1,0}^* \phi_{1,L-1} \right) + H.c. \right] + \frac{U}{2} \hat{n}_{1,0}(\hat{n}_{1,0} - 1) - \mu \hat{n}_{1,0}, \quad (21) $$

$$ \hat{h}_{01} = - \left( J_x \hat{b}^\dagger_{1,1} \hat{b}_{0,1} + H.c. \right) - \left[ J_x \left( \hat{b}_{1,1}^\dagger \phi_{K-1,1} - \phi_{0,1}^* \phi_{K-1,1} \right) + H.c. \right] - \left[ J_y \left( \phi_{0,2}^* \hat{b}_{0,1} - \phi_{0,2} \phi_{0,1} \right) + H.c. \right] + \frac{U}{2} \hat{n}_{0,1}(\hat{n}_{0,1} - 1) - \mu \hat{n}_{0,1}, \quad (22) $$

$$ \hat{h}_{11} = - \left[ J_x \left( \phi_{2,1}^* \hat{b}_{1,1} - \phi_{2,1} \phi_{1,1} \right) + H.c. \right] - \left[ J_y \left( \phi_{1,2}^* \hat{b}_{1,1} - \phi_{1,2} \phi_{1,1} \right) + H.c. \right] + \frac{U}{2} \hat{n}_{1,1}(\hat{n}_{1,1} - 1) - \mu \hat{n}_{1,1}, \quad (23) $$

where the operators and $\phi$ with index ($K - 1$) and ($L - 1$) embody the periodic boundary conditions along $x$ and $y$ directions, respectively. An important point is, with the $2 \times 2$ cluster none of the lattice sites have exact representation of the hopping term. The minimal cluster size which has exact
In total there are sixteen hopping terms with respect to a lattice site is 3 \times 3, and the schematic diagram is shown in Fig. 12. As seen from the figure, the hopping terms involving the central lattice site are represented in green color, are all exact.

For illustration of ED, consider \( N_a = 4 \) and the size of the lattice as 4 \times 4. Then, the number of atoms in \(|\phi\rangle_m\) can range from 0 to 4, and considering that occupation number states at each lattice sites are either \(|0\rangle\) or \(|1\rangle\), the possible row states are:

\[
|0, 0, 0, 0\rangle, |0, 0, 0, 1\rangle, \ldots, |1, 1, 1, 1\rangle.
\]

In total there are sixteen \(|\phi\rangle_m\) and an example of \(|\Phi_c\rangle_\ell\) defined as direct product of four \(|\phi\rangle_m\) is

\[
|\Phi_c\rangle_\ell = |0, 0, 0, 0\rangle \otimes |0, 1, 1, 0\rangle \otimes |0, 0, 0, 1\rangle \otimes |1, 0, 0, 0\rangle.
\]

Thus, the number of \(|\Phi_c\rangle_\ell\) is

\[
M \times N C_{N_a} = 16 \times 4 = 64,
\]

which is much less than the number of states \(2^{16} = 65536\) required for computation with 4 \times 4 cluster in CGMF.

The essence of ED is then to compute the Hamiltonian matrix elements between the cluster states as

\[
\mathcal{H} |\Phi_c\rangle_\ell = \prod_{i=0}^{m'} \prod_{j=0}^{m'} \prod_{k=0}^{M-1} \prod_{l=0}^{N-1} \left( m_k \right) \mathcal{H} [n_i],
\]

and then, diagonalize the Hamiltonian matrix to obtain the eigenvalues and eigenvectors. Considering that the sequence of \(|\Phi_c\rangle_\ell\) is not based on symmetries, but rather based on the combinatorics of \(|\phi\rangle_m\), the row wise computation of Hamiltonian matrix is more efficient. In this regard, the matrix element of the hopping term along \(x\)-axis \( J_x e^{i 2 \pi q a} \hat{b}_{p+1,q} \hat{b}_p \) can be done in the following steps:

1. Compare the row states \(m' |\phi\rangle\) and \(|\phi\rangle_m\) of \(\mathcal{H} |\Phi_c\rangle_\ell\) and \(|\Phi_c\rangle_\ell\), respectively. Proceed to the next step if \(\mathcal{H} |\Phi_c\rangle_\ell\) and \(|\Phi_c\rangle_\ell\) only differ in one of the row states, say the 1st row.

2. Consider \(m' |\phi\rangle\) and \(|\phi\rangle_m\), and compare the single site occupation number states. Proceed to the next step if the difference in these two row states arise from the difference in the occupation number states of two neighbouring lattice sites, say 3rd and 4th lattice sites.

3. The matrix element is nonzero and value is \(\sqrt{n_2(n_2+1)}\) if \(n_2 = n_2 + 1\) and \(n_3 = 3\). For the example considered, we have nonzero matrix element for the term \(p = 2\) and \(q = 1\).

In a similar way, for the example considered, the matrix element of the Hermitian conjugate term \(J_x e^{i 2 \pi q a} \hat{b}_{p+1,q} \hat{b}_p \) is nonzero when the first two conditions are met and the last is modified to \(n_2 = n_2 - 1\) and \(n_3 = n_3 + 1\).

With slight modifications, the same approach can be applied to compute the matrix elements of the hopping term along \(y\)-axis. For this case, two neighbouring row states should be different, and at the level of the lattice sites, the difference should be on the same column. Then, to have nonzero matrix element the occupation numbers should satisfy conditions equivalent of the third condition in the above chain of steps. The computation of the interaction Hamiltonian matrix elements is trivial as it is diagonal and does not require comparison of states.

The general features of the hierarchical definition of states, and the approach to compute the Hamiltonian matrix elements can also be adapted to the CGMF theory as well. As discussed earlier, in the CGMF theory, hopping is exact within the cluster but hopping at the boundary is considered via the mean field \(\phi\). Thus, for cluster of size \(M \times N\), the cluster state defined in Eq. (9) is the direct product of the occupation number states at each lattice site and can be written as

\[
|\Phi_c\rangle_\ell = \prod_{i=0}^{m'} |n_i\rangle,
\]

where \(m' = (M \times N) - 1\) \(i = 0, 1, \ldots, m'\) are the lattice site index, with \(M (N)\) as number of lattice sites along \(x (y)\) direction, \(\ell = \{n_0, n_1, \ldots, n_{m'}\}\) as defined earlier is the index quantum number to identify each of the cluster states uniquely. For illustration, the correspondence between quantum numbers and lattice sites is shown in Fig. 13. The ground state of the CGMF Hamiltonian in Eq. (8) is obtained by using the cluster state in Eq. (25). The Hamiltonian matrix element can be written as

\[
\mathcal{H} |\Phi_c\rangle_\ell = \prod_{j=0}^{m'} \prod_{i=0}^{m'} |n_j\rangle \mathcal{H} |n_i\rangle
\]

\[
= |n_0, n_1, \ldots, n_{m'}\rangle \mathcal{H} |n_0, n_1, \ldots, n_{m'}\rangle.
\]
The definition of the states and computation of the matrix elements can, however, be cast in terms of the row and cluster states as in ED. With this modification, we can implement constraints on the number of atoms in the row and cluster states, thereby reducing the dimension of the Hamiltonian matrix in the CGMF. The only difference from ED is, in CGMF the inter-cluster hopping terms are linear in order parameter \( \phi \) and hence, connect states in Hilbert spaces with different total number of atoms. In other words, the Hamiltonian matrix in CGMF is defined with respect to Fock space. Another difference is, the diagonal terms have contribution from \( \mu \).

![Diagram of a lattice with occupation numbers](image)

**FIG. 13.** The \( M \times N \) cluster with occupation number \( n_0, n_1, \ldots, n_m' \) at each lattice site for CGMF. Each square box represents a lattice site and each of \( n_i \) corresponds to each \( i \) lattice site. Here, \( n_i \) runs from 0 to \( N_0 - 1 \) for each lattice site.

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