Variational study of bosonic phases in two dimensions: fractional Chern insulator, Mott insulator and superfluid

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We numerically study the model wave-functions for a system of hard core bosons at half filling on a square lattice. The candidate wave-functions are based on the projective construction approach \[1\] where a boson is decomposed into two (slave) fermions, each described by a Chern insulator model. Our results confirm that the wave-functions demonstrate the following phases: the superfluid, the Mott insulator and the fractional Chern insulator. In addition, we find that the wave-functions can be continuously tuned from one phase to another by varying the parameters of slave particles. We further propose a microscopic Hamiltonian with a rich phase diagram which variationally supports all the aforementioned phases in different regimes of parameters. The critical behavior across the phase boundaries is investigated and the critical exponents are computed.

Strongly correlated bosons can host various phases of matter such as the superfluid (SF), the Mott insulator (MI) and the fractional quantum Hall (FQH) state (or its lattice version, the fractional Chern insulator (FCI)). It is important to ask whether there is a unifying framework to describe these different bosonic phases and the critical theories associated with their phase transitions. Two places where such a framework is natural is in the context of variational wave-functions and field theory.

The typical approach to representing strongly correlated bosonic phases variationally is by expanding in terms of a product of few-particle distribution functions via Jastrow factors \[2\]. By mapping a classical partition function to the square of the wave-function, it was shown that short-range two-body Jastrow’s were sufficient to capture the qualitative physics of ‘liquid’ and ‘crystal’ phases. Later it was realized that this classical mapping always leads to off-diagonal long range order (ODLRO). Instead, long range-correlations must be introduced in the Jastrow factor to empty the condensate and accurately capture the Mott Insulating phase \[3\]. However, the very fact that these wave-functions are constructed from classical observables makes it difficult to develop a universal scheme to incorporate topologically ordered states such as FQH which are fundamentally quantum.

The projective construction (slave particles) approach is another method to study strongly interacting systems. This approach was largely developed in the context of the spin liquids \[4\] and the FQH in the electronic systems \[5\] and has been applied to study exotic quantum phases such as the exciton bose liquid \[6\]. The underlying idea is to regard the original particles as composite objects which can be fractionalized into slave particles coupled to a gauge field. Compared to the Jastrow wave-functions, this method is directly based on the effective field theory of the target phase. Nonetheless, one needs to carefully treat the emergent fluctuating gauge field in the parton field theory and the question on the stability of a phase can only be addressed by explicitly constructing the wave-functions.

Recently, Barkeshli and McGreevy \[1\] have considered the field theory of the composite bosons in terms of two fermions corresponding to topological bands with non-zero Chern numbers. At the mean-field level, all three aforementioned bosonic phases may be stabilized for certain choices of Chern numbers. In case of FQH, this theory is equivalent to the composite fermion picture \[7\] once one of the slave fermions is integrated out. In this letter, we go beyond the mean-field theory by explicitly constructing the projected wave-functions. We set up a microscopic Hamiltonian for the slave particles and identify the phase represented by each wave-function. We compute the single-particle density matrix (Fig. 2(a)) and its eigenspectrum (Fig. 2(b),(c)) to establish the ODLRO in SF. We calculate the structure factor (Fig. 2(d)) where the SF-MI or FCI-MI transitions manifest themselves as a jump in the slope. The MI wave-functions has a clear diagonal long-range order (DLRO) in absence of any ODLRO. We show that the \( \nu = 1/2 \) FCI trial wave-
function is doubly degenerate on torus (Fig. 3) and has a quantized Hall conductance of $1/2$. These methods are much more accurate compared to the ones based on the topological entanglement entropy. The simulated phase diagram is summarized in Fig. 1(left) and is in agreement with the mean-field phase diagram.

Inspired by the form of the parton Hamiltonian, we examine a microscopic model Hamiltonian for bosons. This model is an extended version of the Bose-Hubbard model with nearest neighbor interactions and frustrated next nearest neighbor hopping terms that can in turn be interpreted as a result of a $2\pi$ magnetic flux per plaquette. We map out the phase diagram of this model (Fig. 1(right)) and variationally show that all three phases can emerge in different regimes of parameters. The critical exponents are also derived (see Tab. I). In case of SF-MI, we have found a good agreement with the known critical value as well as the critical exponents.

**Projective Construction**— We study a system of hard core bosons on a square lattice at half filling. Following the prescription of [11], we define the fermionic representation of the charge one bosons by $b^\dagger_i = f^\dagger_{1,i} f^\dagger_{2,i}$ where $f_{1,i}$ and $f_{2,i}$ correspond to two different flavors of charge one-half fermions and $i$ labels the lattice site. This construction enlarges the Hilbert space and the constraint $b_i^\dagger b_i = f_{1,i}^\dagger f_{1,i} = f_{2,i}^\dagger f_{2,i}$ must be imposed. We consider the mean-field Hamiltonian [8] that breaks the SU(2) symmetry in parton-space to U(1)

$$H = \sum_{\alpha,i,j} t_{\alpha,i,j} e^{i\left(A_{\alpha}/2 - q_{\alpha} a_{\alpha}(i)\right)} f^\dagger_{\alpha,i} f_{\alpha,j}$$

$$+ \left(A_{0}(i)/2 - q_{a} a_{0}(i)\right) \delta_{ij} f^\dagger_{\alpha,i} f_{\alpha,i}$$

(1)

where $A_{\mu} = (A_{0}, \widetilde{A})$ is the external gauge field, $\alpha = 1, 2$ labels the fermion flavor, and $q_{1(2)} = \pm 1$ are the corresponding internal gauge charge of $f_{1(2)}$. The hopping amplitudes $t_{\alpha,i,j}$ play the role of Hubbard Stratonovich fields which are static up to a fluctuating phase $a_{ij}$. The Lagrange multiplier $a_{0}(i)$ is introduced to ensure the particle number constraint. The combination of these fields $a_{\mu} = (a_0, \widetilde{a})$ therefore leads to an emergent local U(1) gauge symmetry.

As a choice of $t_{\alpha,i,j}$ parameters, we consider the $\pi$-flux square lattice model [11] for both $f_1$ and $f_2$ fermions with three parameters for each [8]: nearest neighbor hopping ($t_0$), next nearest neighbor hopping ($\Delta_0$) and the on site mass term ($m_\alpha$) where $\alpha = 1, 2$ indicates the corresponding parameter for $f_1$ and $f_2$ respectively. The spectrum of this model is gapped at half filling and the Chern number associated with the filled bands can be tuned by varying the above parameters. We fix the Hamiltonian for $f_1$: $t_1 = 2\Delta_1 = 2$ and $m_1 = 0$ giving the lowest band unit Chern number $C_1 = 1$. Consequently, the phase diagram can be derived in terms of the $f_2$ parameters; i.e. $\Delta_2$ and $m_2$, see Fig. 1(left) or Tab. I. The bosonic wave-function is a projected product of two slater determinants

$$\Psi(\{r_i\}) = \det_1(\{r_i\}) \times \det_2(\{r_i\})$$

(2)

where the projection simply means the same configuration $\{r_i\}$ for both fermions.

We use variational Monte-Carlo to characterize the candidate wave-functions. Note that the wave-functions are constructed based on the $\pi$-flux Hamiltonian and they are complex-valued in general. Deep in the SF phase ($m_2 = 0$) the phases of the slater determinants exactly cancel each other and the resulting wave-function is real. This is indeed consistent with the flux smearing argument in the composite fermion picture [7, 12]. As we deviate from $m_2 = 0$ towards the MI phase some configurations acquire a phase. However, we find that $\langle b^\dagger_{\alpha} b_{\beta}\rangle$, $\langle n_{\alpha} n_{\beta}\rangle$ and variational energy only weakly depend on the phase angle of the wave-function and one can safely take the modulus or the real-part. We also note that the FCI

| $f_2$ parameters | $C_2$ bosonic phase |
|-----------------|---------------------|
| $\Delta_2 > 0$, $|m_2| < 4|\Delta_2|$ | +1 FCI $\nu = 1/2$ |
| $\Delta_2 < 0$, $|m_2| < 4|\Delta_2|$ | −1 SF |
| $|m_2| > 4|\Delta_2|$ | 0 MI |

TABLE I. The bosonic phases in terms of the $f_2$ Chern number, $C_2$, while the $f_1$ Chern number is fixed at $C_1 = 1$. The scale is set by $t_2 = t_1 = 2$.  

FIG. 2. (a), (b) The entanglement spectrum of SPDM $\chi(r, r')$ as a function of $m_2$. (c) SPDM $\chi(|r - r'|)$ for different values of $m_2$ along path(2) in Fig. 1(left). SF-MI transition as a change from the power law to the exponential decay is evident. (d) The evolution of $S(q)/|q|$ as $m_2$ tuned across SF/FCI-MI transition. Different colors from top to bottom represent $m_2 = 0, 1, 6, 3, 2, 3.9, 4.8, 6.4, 8$. Solid lines in (c) and (d) are fits. Errorbars are smaller than the symbols. The system size is $16 \times 16$. 


wave-functions is equal to the SF wave-function times an extra phase angle which is responsible for the topological order. This is a property of Laughlin wave-functions \[13\] and this observation supports the idea that our wave-function is in fact a lattice version of the Laughlin state.

**Single-particle density matrix (SPDM)—** We first calculate the bulk (SPDM) \(\chi(r, r') = \langle b_r^\dagger b_{r'}\rangle\) to search for ODLRO. To see how SPDM behaves in different phases we take two paths in the phase diagram shown by the arrows in Fig. 1(left). We observe that in both FCI and MI phases SPDM always decays exponentially \[3\] which means the quasi particle spectrum in these two states are gapped. However, in the SF phase the SPDM assumes a power law \(1/r^\alpha\) where \(\alpha = 0.95 \pm 0.05\) consistent with \(\alpha = 1\) in the previous studies of the superfluidity in 2+1D bosonic systems \[14\]. The transition from a power law behavior to an exponential decay occurs at the critical value \(m_2 = 4\Delta_2\), at which \(C_2\) changes from \(-1\) to 0 (see Fig. 2(c)). We represent the zero momentum (condensate) population \(n_0 = \langle b_r^\dagger b_r\rangle\) by a color code to reconstruct the left half of the phase diagram in Fig. 1(left). The agreement with the mean-field theory is quite remarkable.

We further use SPDM to establish the fact that the quasi particles in FCI and MI states are distinct in character: one is localized on the lattice sites (solid) and the other is delocalized over the lattice (fluid). To this end, we look at the entanglement spectrum of SPDM

\[
\chi(r, r') = \sum_\ell n_\ell \phi_\ell^*(r)\phi_\ell(r')
\]

where \(\phi_\ell(r)\) (natural orbital) is the right eigenstate of SPDM with the eigenvalue \(n_\ell\). This decomposition procedure is well-known as a conventional probe which identifies a Bose-Einstein condensate (BEC) \[13\] when one of \(n_\ell\)'s is macroscopically occupied. We verify this in the SF phase (see Fig. 2(a)). Deep in the MI, the spectrum is accumulated only at zero and one (i.e. particles fully localized on the lattice sites). In contrast, the spectrum in FCI is almost continuous between zero and one, showing the particle wave-functions are delocalized (Fig. 2(b)).

**Structure factor—** To detect DLRO, we study the static structure factor which is defined by

\[
S(q) = \langle n_q n_{-q}\rangle = \frac{1}{N} \sum_{r, r'} e^{-iq \cdot (r-r')} \langle n_r n_{r'}\rangle
\]

where \(N\) is the number of sites and \(n_r = b_r^\dagger b_r\) is the particle number operator. As mentioned earlier, the wave-functions of SF and FCI are identical in modulus and therefore have the same structure factor. The evolution of the structure factor in the low-\(q\) limit is illustrated in Fig. 2(d). There is a jump at the critical point \((m_2 = 4\Delta_2)\) of the SF/FCI-MI transitions in accordance with the earlier results. Furthermore, there is a peak in the MI phase at \(q = (\pi, \pi)\) corresponding to the checker board charge density wave (CDW) structure. This type of configuration is determined by the mass term which enlarges the unit cell in the parton Hamiltonian \[8\] and should not be considered as a spontaneous breaking of the translational symmetry. Recently, a different field theory \[10\] that does incorporate spontaneous lattice translation symmetry breaking was developed.

**Topological properties—** For further wave-function characterization, we concentrate on the gapped phases and consider their topological properties. We calculate the topological degeneracy on a torus, Hall conductance and topological entanglement entropy (TEE) (see \[8\] for latter). However, we note that, because of finite size effects, the two former methods are much more accurate. To determine the degeneracy of the ground state, we study the change in the wave-function as a \(2\pi\) flux quantum is inserted into either hole of the torus. We introduce the twisted boundary conditions associated with an external field

\[
\langle r + L_x \hat{x}|\Psi(\bar{\theta}_\gamma, \gamma)\rangle = e^{i\gamma_x} \langle r|\Psi(\bar{\theta}_\gamma, \gamma)\rangle
\]

\[
\langle r + L_y \hat{y}|\Psi(\bar{\theta}_\gamma, \gamma)\rangle = e^{i\gamma_y} \langle r|\Psi(\bar{\theta}_\gamma, \gamma)\rangle
\]

where a bosonic many-body wave-function with an external twist angle \(\gamma = (\gamma_x, \gamma_y)\) is denoted by \(|\Psi(\bar{\theta}_\gamma, \gamma)\rangle\) and \(L_x \times L_y\) is the system size. Note that the \(\bar{\theta}\) is a static internal twist angle and can be found as the stationary
solution of the effective action \[8\]

\[
\tilde{\theta}_\gamma = \left( \frac{C_1 - C_2}{C_1 + C_2} \right) \frac{\gamma}{2}
\]

This contribution to the twist angle from the internal gauge field must be included in the parton Hamiltonian for computing the Slater determinants; otherwise this method yields incorrect results \[8\]. We compute the inner product matrix of four possible wave-functions

\[
N(\gamma, \gamma') = \langle \Psi(\tilde{\theta}, \gamma) | \Psi(\tilde{\theta}, \gamma') \rangle
\]

where \(\gamma = (0, 0), (0, 2\pi), (2\pi, 0)\) and \((2\pi, 2\pi)\). The rank of this matrix yields the dimension of the ground state space. The normalized eigenvalues of \(N(\gamma, \gamma')\) determine the weight of the corresponding eigenstate. As shown in Fig. 3, there are two independent eigenstates with 0.5 weight in FCI where the local density matrix is identical; in contrast, in the MI phase there is only one dominant eigenstate which implies that there is no degeneracy. By comparing the local density matrices, we also checked that the remaining weight in the eigenspectrum of the MI phase is locally distinguishable from the dominant eigenstate (see inset of Fig. 3(b)). In the appendix \[8\], we present an alternative method to compute the topological degeneracy purely based on the internal gauge field \(a_\mu\).

The Hall conductance of a many body wave-function is given in terms of the Chern number \(C\) \(\sigma_{xy} = C e^2/h\). We show that \(C = 0.50 \pm 0.01\) per each state in FCI and \(C = 0.0 \pm 0.01\) in MI. The Chern number of a non-degenerate many-body wave-function is computed in terms of an integration of the adiabatic curvature over the space of twisted boundary conditions \[8\].

**Microscopic Hamiltonian**—Given these variational ansatz, one can ask if there is a microscopic Hamiltonian which support the three phases. We consider an extension of the Bose-Hubbard model given by

\[
H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + r \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) \\
+ \frac{U}{2} \sum_{\langle i,j \rangle} n_i n_j
\]

where \(U\) is the nearest neighbor interaction and the hard-core limit is assumed. The nearest neighbor hopping \((-t)\) is negative while the next nearest neighbor (diagonal) hopping \((r)\) is positive. This model can be viewed as a physical model (originally with all negative hopping amplitudes) subject to a 2π flux per plaquette. The large-\(U\) limit favors the MI state. In the small-\(U\) limit, \(r \ll t\) gives SF with a condensate at \(k = 0\) and \(r \ll t\) leads to SF with a condensate at \((0, \pi)\) or \((\pi, 0)\). We find the FCI phase emerges between these two extreme limits.

To see this, we optimize the variational energy \(E = \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle\) in \((m_2, \Delta_2)\)-space of the trial wave-functions \[17\] for each value of \((r/t, U/t)\) and map out the phase diagram of Fig. 1(right). We compute the critical exponents and the anomalous dimension \(\langle b_i^\dagger b_j + b_j^\dagger b_i \rangle \propto 1/r^{1+\eta}\) for the SF-MI and SF-FCI transitions \[8\]. The results are summarized in Tab. 1. For SF-MI transition, the calculated critical value of \(t/U\) is very close to other numerical studies \[9, 10\] as well as the analytical results \[18\]. Our finding for the critical exponent \(\xi \sim |t - t_c|^{-\nu}\) agrees with the predicted value of \(\nu = 2/3\) corresponding to the 3D XY-model \[12, 19\]. Overall in both SF-MI and SF-FCI transitions, the evaluated anomalous dimension is rather large and in the case of SF-MI our result appears to be far from \(\eta = 1/5\) as expected for the 3D XY-model \[12\]. This deviation could be the result of finite size systems. We observe that the FCI-MI transition does not show the critical scaling behavior; in other words, the correlation length shows a discontinuity at the critical point instead of diverging to infinity \[8\]. This behavior could be due to finite size effects. Two remarks are in order. We should note that FCI wave-function is not real for all configurations while the true ground state of Eq\[8\] has to be real. However, all the correlation functions we have computed are real and the variance of the variational energy \[8\] is relatively small. These observations strongly support the idea that the FCI wave-function and the true ground state could be adiabatically connected. Another remark is that the Hamiltonian of Eq\[8\] can be mapped into an extended version of the frustrated XXZ-model where the intermediate regime of \(r/t\) could host a spin-liquid (SL) phase. Given the equivalence of FCI and the chiral SL, our results signals a possibility of realizing a chiral SL in this model. These questions will be a subject of a future work.

In conclusion, we present a unifying scheme for constructing the candidate wave-functions to describe SF, MI and FCI phases. The variational parameters can be tuned to transition from one phase to another. Finally, we have introduced a microscopic Hamiltonian which variationally supports all the phases and allows for direct transitions between them.

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