Superfluid-insulator transition of ultracold bosons in an optical lattice in the presence of a synthetic magnetic field

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Abstract – We study the Mott-insulator–superfluid transition of ultracold bosonic atoms in a two-dimensional square optical lattice in the presence of a synthetic magnetic field with \( p/q \) (\( p \) and \( q \) being co-prime integers) flux quanta passing through each lattice plaquette. We show that on approach to the transition from the Mott side, the momentum distribution of the bosons exhibits \( q \) precursor peaks within the first magnetic Brillouin zone. We also provide an effective theory for the transition and show that it involves \( q \) interacting boson fields. We construct, from a mean-field analysis of this effective theory, the superfluid ground states near the transition and compute, for \( q = 2, 3 \), both the gapped and the gapless collective modes of these states. We suggest experiments to test our theory.

The physics of ultracold bosonic atoms in an optical lattice can be well described by the Bose-Hubbard model [1,2]. In fact, experiments on the Mott-insulator–superfluid (MI-SF) transitions of such bosonic atoms in two-dimensional (2D) optical lattices [3] is found to agree with predictions of theoretical studies of the Bose-Hubbard model quite accurately [4–6]. More recently, there has been several theoretical proposals of generating both Abelian and non-Abelian artificial vector potentials for bosonic or fermionic neutral atoms [7]. Following such suggestions, several experiments have successfully generated time- or space-dependent effective vector potentials for these neutral bosonic atoms by creating temporally or spatially dependent optical coupling between their internal states [8,9]. Such a generation of synthetic space-dependent vector potential and hence magnetic fields is complementary to the conventional rotation technique [10]. Several theoretical studies have also been carried on the properties of the bosons in an optical lattice in the presence of an effective magnetic field [11]. In particular, the MI-SF phase boundary has been computed using mean-field theory [12] and excitation energy calculation using a perturbative expansion in the hopping parameter [13]. However, experimentally relevant issues such as the momentum distribution of the bosons in the Mott phase, the critical theory of the MI-SF transition, and the nature of the superfluid ground states and collective modes near criticality have not been addressed so far.

In this letter, we present a theory of the MI-SF transition for ultracold bosons in a 2D square optical lattice with commensurate filling \( n_0 \) and in the presence of a synthetic vector potential corresponding to \( p/q \) (\( p \) and \( q \) are co-prime integers) flux quanta per plaquette of the lattice which addresses all of the above-mentioned issues. The novel results of our work which have not been addressed in earlier studies are as follows. First, using a strong-coupling RPA theory for the bosons [5], we provide an analytical formula for their momentum distribution in the Mott phase and show that it develops \( q \) precursor peaks on approach to the MI-SF transition. Second, based on both the microscopic strong-coupling theory and a symmetry analysis, we construct the critical field theory for the transition and show that it necessarily involves \( q \) coupled boson fields [14]. Third, using a mean-field analysis of this effective theory, we find the superfluid ground state to which the transition takes place and chart out the corresponding spatial patterns of the condensate density. Finally, we compute the collective modes of the superfluid phase for \( q = 2, 3 \), explicitly demonstrating the

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nature of both the gapped and gapless collective modes near the transition, and provide analytical expressions for their masses and group velocities in terms of microscopic parameters of the theory. We suggest realistic experiments which can verify specific predictions of our theory.

The Hamiltonian of a system of bosons in the presence of an optical lattice and a synthetic magnetic field is given by [1,3,4,12,13]

\[ H = \sum_{r,r'} J_{rr'} \hat{b}_r \hat{b}_{r'} + \sum_r \left[ -\mu \hat{n}_r + \frac{U}{2} \hat{n}_r(\hat{n}_r - 1) \right], \tag{1} \]

where \( J_{rr'} = -J \exp(-i q^* \int_0^\beta A^* \cdot \vec{A} \cdot \vec{A} / \hbar c) \), if \( r \) and \( r' \) are nearest neighboring sites and zero otherwise, \( A^*(0,\alpha) \) is the effective charge (magnetic field) for the bosons, \( J \) is the hopping amplitude determined by the depth of the optical lattice, and the value of \( q^*B^* \) can be controlled by varying the detuning between the hyperfine states of the bosonic atoms [9]. Here \( \mu \) is the chemical potential, \( U \) is the on-site Hubbard interaction, and \( \hat{n}_r (\hat{b}_r \hat{b}_r^\dagger) \) is the boson annihilation (density) operator. In the rest of this work, we consider the magnetic field to correspond to \( p/q \) flux quanta through the lattice: \( q^*B^* / \hbar c = 2\pi p/q \), and set the lattice spacing \( a \), \( \hbar \), and \( c \) to unity.

The effective action manifests itself in the first term of eq. (1) and thus vanishes in the local limit \( (J=0) \). In this limit the boson Green function at \( T=0 \) can be exactly computed [2,5,6]:

\[ G_0(\omega_n) = \frac{n_0 + 1}{i \omega_n - E_p} - \frac{n_0}{i \omega_n + E_h}. \tag{2} \]

Here \( \omega_n \) denote bosonic Matsubara frequencies and \( E_h = \mu - U(n_0 - 1)(E_p = -\mu + U n_0) \) are the energy cost of adding a hole (particle) to the Mott state. To address the effects of the hopping term, we write down the coherent state path integral corresponding to \( \mathcal{H} \):

\[ S = \int_0^\beta d\tau \left[ \sum_r \bar{\psi}_r^\dagger(\tau) \dot{\psi}_r(\tau) + \mathcal{H}[\psi^*, \bar{\psi}] \right], \tag{3} \]

\( \tau \) is the imaginary time, \( \beta = 1/k_B T \) is the inverse temperature \( (T) \), and \( k_B \) is the Boltzmann constant. Following ref. [5], we then decouple the hopping term by two successive Hubbard-Stratonovitch transformations, integrate out the original boson and the first Hubbard-Stratonovitch fields, and obtain the final form of the strong-coupling effective action \( S_{\text{eff}} = S_0 + S_1 \)

\[ S_0 = \int \bar{\psi}_r^\dagger(\omega_n, \mathbf{k})[-G_0^{-1}(\omega_n)I + J_q(\mathbf{k})] \psi_r(\omega_n, \mathbf{k}), \]

\[ S_1 = g/2 \int_0^\beta d\tau \int d^2r [\bar{\psi}_r^\dagger(\mathbf{r}, \tau) \psi_r(\mathbf{r}, \tau) - \mu \bar{\psi}_r(\mathbf{r}, \tau)], \tag{4} \]

where \( \psi_r(\mathbf{r}, \tau) = (\psi(0, \mathbf{k}_x, \mathbf{k}_y), \ldots \psi_{q-1}(k_x, \mathbf{k}_y))^T \) with \( \psi_n(k_x, \mathbf{k}_y) = \psi(k_x + 2\pi n/q, \mathbf{k}_y) \) denotes the \( q \)-component auxiliary field introduced through the second Hubbard-Stratonovitch transformation and have the same correlation functions as the original boson fields \( \bar{\psi}^\dagger, \psi^\dagger \) and \( J_q(\mathbf{k}) \) is the effective hopping term for \( q \) bosons. To evaluate \( J_q(\mathbf{k}) \) is the consequence of \( q \) fold degeneracy of the magnetic Brillouin zone \( (\pi / q < k_x < \pi, \ldots) \).

\[ J_q = (1/\beta) \sum_{\omega_n} \int d^2k/(2\pi)^2, \]

\( I \) denotes the unit matrix, and \( g > 0 \) is the static limit of the exact two-particle vertex function of the bosons in the local limit [5]. Here \( J_q(\mathbf{k}) = [G_0^{-1}(\omega_n)I + J_q(\mathbf{k})]^{-1} \) amounts to inverting \( J_q(\mathbf{k}) \).

The critical hopping \( J_c \) for the MI-SF transition as a function of \( \mu \) can be determined from the condition [2]

\[ r_q = -G_0^{-1}(\omega_n = 0) + \epsilon_q^m(\mathbf{k} = \mathbf{Q}^m) = 0. \tag{5} \]

The MI-SF phase boundary so obtained is shown in fig. 1 for \( q = 2 \) and agrees qualitatively with those obtained using mean-field theory [12] and \( J/\mu \) expansion [13]. The inset shows variation of \( J_c / U \) at the tip of the \( n_0 = 1 \) Mott lobe displaying monotonic decrease (non-monotonic behavior) at large (small) \( q \) as also found in ref. [12].

Having compared the phase diagram obtained by our method with other methods available The consequence of the \( q \) fold degeneracy of \( \epsilon_q^m \) becomes evident in the momentum distribution of the bosons in the Mott phase,
which, at \( T = 0 \), is given by

\[
n(k) = -\lim_{\nu \to 0} (1/\beta) \sum_{\omega_n} \text{Tr} G(i\omega_n, k) \exp(i\omega_n 0^+) = \sum_{\alpha=0...q-1} E^{\alpha+}_q(k) + \delta \mu + U x E^{\alpha-}_q(k) - E^{\alpha-}_q(k),
\]

where \( \delta \mu = \mu - U(n_0 - 1/2) \), \( x = (n_0 + 1/2) \) and

\[
E^{\alpha\pm}_q(k) = \frac{1}{2} \left[ -2\delta \mu + \epsilon^x_q(k) \pm \sqrt{\epsilon^x_q(k)^2 + 4\epsilon^y_q(k) U x + U^2} \right]
\]

(6)

(7)

denotes the position of the poles of \( G(k, i\omega_n) \) in the Mott phase. Note that \( E^\alpha_q \) can also be obtained from a time-dependent variational method [16].

Equation (6) is a central result of this work and generalizes its counterpart in ref. [5] in the presence of a magnetic field. The peaks of \( n(k) \) occur when \( E^{\alpha+}_q(k) - E^{\alpha-}_q(k) \) becomes small near the MI-SF transition. The degeneracy of \( E^\alpha_q \) and hence \( E^{\alpha\pm}_q \) ensures that this happens at \( q \) points in the first Brillouin zone leading to \( q \) precursor peaks in \( n(k) \) at \( k = Q^\alpha \). This is demonstrated in Fig. 2 for \( q = 2 \) and \( q = 4 \). Note that the positions of these peaks in the Brillouin zone depend on the specific form of the vector potential realized in the experiments; for symmetric vector potentials generated by rotation they would appear at \( (\pi \alpha/q, \pi \alpha/q) \). However, their number depends only on \( q \) and the lattice geometry. We point out that the apparent “gauge dependence” of \( n(k) \) is a direct consequence of the realization of a specific vector potential (and not field which can be represented by all gauge-equivalent vector potentials) in experimental setups and does not contradict any fundamental principle.

At \( J_c \), the MI-SF transition occurs since the energy gap to addition of particles and/or holes to the Mott state vanishes. In contrast to standard superfluid-insulator transition [4–6], the presence of \( q \) degenerate minima at \( k = Q^\alpha \) necessitates the corresponding Landau-Ginzburg theory to be constructed out of \( q \) low-energy fluctuating fields \( \phi^\alpha(r, t) \) around these minima:

\[
\psi_q(r, t) = \sum_{\alpha=0...q-1} \chi^\alpha_q(r) \phi^\alpha(r, t),
\]

(8)

where \( \chi^\alpha_q(r) \) denotes the eigenvectors of \( J_q(Q^\alpha) \) in real space, and we have Wick-rotated to real time. The quadratic part of the Landau-Ginzburg theory, obtained by expanding \( S_0 \) (eq. (4)) about the minima, is given by

\[
S_0 = \int d^2 r dt \sum_{\alpha=0...q-1} \phi^{\alpha+}(r, t) [K_0 \partial_t^2 + i K_1 \partial_t + r_q - v_q^2 (\partial_x^2 + \partial_y^2)] \phi^\alpha(r, t),
\]

(9)

where the parameters \( K_0, K_1 \) and \( v_q \) are given by

\[
K_0 = 1/2 \partial^2 G_0^{-1}/\partial \omega^2|_{\omega = 0} = n_0(n_0 + 1) U^2 / (\mu + U)^3, \]

\[
K_1 = \partial G_0^{-1}/\partial \omega|_{\omega = 0} = 1 - n_0(n_0 + 1) U^2 / (\mu + U)^2, \]

\[
v_q^2 = \nabla^2 \epsilon^m_q(k)/2, \quad v_q^2 = J/\sqrt{2}.
\]

At the tip of the Mott lobe, where \( \mu = \mu_{tip} = U (\sqrt{n_0(n_0 + 1) - 1} \), \( K_1 = 0 \). Thus we have a critical theory with dynamical critical exponent \( z = 1 \). Away from the tip, \( K_1 \neq 0 \) rendering \( z = 2 \) [2].

The most general quartic Landau-Ginzburg action in terms of \( q \) bosonic fields which is allowed by invariance under projective symmetry group (PSG) of the underlying square lattice has been obtained in ref. [14]. The elements of the PSG for the square lattice include translation along \( x \) and \( y \), rotation by \( \pi/2 \) about the \( z \)-axis, and reflections about the \( x \) and \( y \) axes. The transformation properties of \( \phi^\alpha \) fields under these operations are tabulated in ref. [14].

The invariant quartic action so obtained is given by

\[
S_1 = \frac{1}{4} \int d^2 r dt \sum_{\alpha, \beta, \gamma=0} \Gamma^\alpha_{\beta\gamma} \phi^\alpha \phi^{\alpha+} \phi^\beta \phi^{\beta+} \phi^\gamma \phi^{\gamma+},
\]

(11)

where \( \Gamma^\alpha_{\beta\gamma} = \Gamma^-_{\alpha\beta\gamma} = \Gamma^\alpha_{\beta\gamma} = \Gamma^\alpha_{\gamma\alpha\beta} = \Gamma^\alpha_{\alpha\beta\gamma} \) and sums over integers \( \alpha, \beta, \gamma \) are taken modulo \( q \). Equation (9) along with \( S_1 \) has been analyzed in details in ref. [14]. However, the lack of microscopic knowledge of \( \Gamma^\alpha_q \) did not allow identification of the exact ground state of \( S_1 \); only possible symmetry-allowed ground states were charted.

Here, taking advantage of the microscopic knowledge of \( q \) and \( \chi^\alpha_q \), we determine the exact superfluid state to which the transition takes place. This is done by substituting of eq. (8) in eq. (4) followed by coarse-graining of the resultant action which involves replacing \( \chi^\alpha_q \) by its sum over \( q \) lattice sites:

\[
\int d^2 r dt \int \chi^\alpha_q(r) L_1 \phi^\alpha(q, r, t) \to \left\{ (1/q^2) \sum_{x,y=0}^{q-1} L_1[\chi^\alpha_q(r)] \right\}
\]

\[
\times \int d^2 r dt \int \phi^\alpha(r, t) \to c \int d^2 r dt \int \phi^\alpha(r, t).
\]

Here \( L_1 \) and \( L_2 \) denotes arbitrary fourth order polynomial functions and the coarse-graining procedure is applicable due to the natural separation of scale between the spatial variation of \( \chi^\alpha_q(r) \) and \( \phi^\alpha(q, r, t) \). The effective action so obtained is then compared to \( S_1 \) to obtain \( \Gamma^\alpha_{q\beta} \). Finally,
we minimize the resultant action at the mean-field level and obtain the superfluid ground state near the MI-SF transition. This procedure is most easily demonstrated for $q = 2$. Here, $\epsilon_0^q(k) = -2J\sqrt{\cos^2(k_x^0) + \cos^2(k_y^0)}$ leading to two minima at $(k_x, k_y) = (0, 0)$ and $(\pi, \pi)$ with eigenfunctions

$$\chi_0^q(r) = (1 + \sqrt{2} + \exp(ipx))/\sqrt{4 + 2\sqrt{2}},$$

$$\chi_1^q(r) = \exp(ipy)(1 + \sqrt{2} - \exp(ipx))/\sqrt{4 + 2\sqrt{2}}.$$  \hspace{1cm} (12)

Putting these values in eq. (8) and eq. (4), the coarse-grained effective action reads

$$S^{q=2}_{\text{eff}} = \frac{1}{8} \int d^2 r \left[ 3g(|\phi^0(\mathbf{r}, t)|^2 + |\phi^1(\mathbf{r}, t)|^2)^2 + g(\phi^{0\ast}(\mathbf{r}, t)\phi^0(\mathbf{r}, t) - \phi^{1\ast}(\mathbf{r}, t)\phi^0(\mathbf{r}, t))^2 \right].$$ \hspace{1cm} (13)

Comparing $S^{q=2}_{\text{eff}}$ with $S_1$ for $q = 2$, we find $\Gamma_0^q = 3g/2$ and $\Gamma_1^q = g/2$. A mean-field analysis then yields the superfluid ground state: $\langle \phi^0(\mathbf{r}, t) \rangle = \phi^0 = i\phi^1 = \phi^1(\mathbf{r}, t)$. The renormalized condensate density can be obtained by using $\rho_0^{(2)}(\mathbf{r}) = |\psi_{\text{MF}}^0(\mathbf{r})|^2$, where $\psi_{\text{MF}}^0$ is obtained by substituting $\langle \phi^0(\mathbf{r}, t) \rangle$ in eq. (8). Analogous procedure carried out for $q = 3$ yields the superfluid ground state: $\langle \phi^0(\mathbf{r}, t) \rangle = 0$, $\langle \phi^1(\mathbf{r}, t) \rangle = 0$. The resultant plots of $\rho_0^q(\mathbf{r})$, shown in fig. 3 for $q = 2$ and $q = 3$, display 2 and 3 sublattice patterns, respectively. We note that the procedure mentioned above constitutes a general method for obtaining the superfluid ground state and density near the MI-SF critical point for any $q$.

Finally, we compute the collective modes of the superfluid ground state near the transition. First we consider the case $q = 2$ and rewrite $S^{(2)}_{\text{eff}}$ in terms of a linear combination of the $\phi^q$ fields: $\xi^{(1)} = (\phi^0 + [-i\phi^1])/\sqrt{2}$. The quartic action becomes

$$S^{q=2}_{\text{eff}} = \frac{1}{8} \int d^2 r \, dt [3g(|\xi^0(\mathbf{r}, t)|^2 + |\xi^1(\mathbf{r}, t)|^2)^2 + g(|\xi^0(\mathbf{r}, t)|^2 - |\xi^1(\mathbf{r}, t)|^2)^2],$$ \hspace{1cm} (14)

so that the superfluid ground state corresponds to condensation of $\xi^0$. The quadratic action can be written as

$$S_0^q = \int \frac{d^2 k \, d\omega}{(2\pi)^2} \sum_{\alpha=0}^{q-1} \xi^{\ast}(\mathbf{k}, \omega) [-G_0^{-1}(\omega) - 2v_2^2|\mathbf{k}|^2] \xi^\alpha(\mathbf{k}, \omega),$$ \hspace{1cm} (15)

with $c_2 = -c_2(k = 0) = 2\sqrt{2}J$. Using these actions, and carrying out a straightforward linearization $\xi^0(\mathbf{r}, t) = \xi^0 + \delta^0(\mathbf{r}, t)$ and $\xi^1(\mathbf{r}, t) = \delta^1(\mathbf{r}, t)$, where $\xi^0 = \sqrt{2}\lambda_1|\mathbf{r}|/g$, we find that there are four collective modes. Two of these correspond to the condensed field $\xi^0$ and $\xi^{\ast 0}$, and have dispersions

$$\omega^{(1)}_{\pm} = \pm \frac{\sqrt{2}}{2} \left( \frac{D_2(k)}{2} + \frac{D_4(k)}{4} - C_2(k)^{1/2} \right)^{1/2},$$ \hspace{1cm} (16)

$$B_2(k) = 2h - A_2(k)^2 + 2a_0(v_2 \mathbf{k}^2 - r_2) - r_2^2,$$ \hspace{1cm} (17)

$$C_2(k) = a_0^2 v_2^2 |\mathbf{k}|^2 (v_2^2 |\mathbf{k}|^2 - 2r_2),$$ \hspace{1cm} (18)

$$A_2(k) = -c_2 + v_2^2 |\mathbf{k}|^2 - r_2,$$ \hspace{1cm} (19)

where $a_0 = (U + \mu)$. At low wave vector, $\omega^{(1)}_+$ is gapped with a mass $m_1 = \sqrt{B_2(0)}$ while $\omega^{(1)}_-$ has linear dispersion with velocity $v_2 = v_2a_0\sqrt{2|r_2|/m_1}$. The other two modes, which correspond to the non-condensed field $\chi^1$ and $\chi^{\ast 1}$, have dispersions

$$\omega^{(2)}_{\pm} = \pm \frac{D_2(k)}{2} + \frac{D_4(k)}{4} + a_0 \left( \frac{|r_2|}{2} + v_2^2 |\mathbf{k}|^2 \right)^{1/2},$$ \hspace{1cm} (20)

$$D_2(k) = -(2\delta^0 + c_2 - v_2^2 |\mathbf{k}|^2 + r_2/2).$$
Both these modes are gapped in the superfluid phase with masses

\[ m_{2[3]} = \pm \frac{1}{2} D_2(0)+\frac{\sqrt{D_2(0)^2/4+\alpha_0|r_2|}}{2}. \]  

(21)

The masses \( m_{1,2,3} \) and the velocity \( v_G \) of these modes, plotted as a function \( \mu \) in fig. 4 for several representative values of \( J/J_c \), displays the following characteristics. At \( \mu = \mu_{tip} \) and \( J = J_c \), where \( 2\delta \mu = -c_2 \) rendering \( D_2(0) = 0 \) and \( D_3(0) = 0 \), all the modes become gapless with \( \omega = |k| \) dispersion. Also at \( \mu \neq \mu_{tip} \), one of the two modes \( \omega_{\pm}^{(2)} \) always remain gapless at \( J = J_c \) with \( \omega = |k|^2 \) dispersion. The velocity \( v_G \) at \( J = J_c \), is non-zero only at \( \mu = \mu_{tip} \); thus it shows a peak at \( \mu_{tip} \) for \( J \) close to \( J_c \). We emphasize that our theory specifies \( v_G \) and \( m_{1,2,3} \) in terms of the parameters of the Bose-Hubbard model.

For \( q = 3 \) only \( \phi^0 \) condense, and the corresponding collective modes are given by eq. (16) with \( c_2, c_3, r_2 \rightarrow c_3, v_3, r_3 \) (where \( c_3 = -c_3^{(0)}(0) \)). This leads to similar gapped and a gapless mode with linear dispersion as for \( q = 2 \). However, the dispersion of the non-condensed modes are different. The effective action \( S_{eff}^{q=3} \) turns out to be \( O(3) \) symmetric:

\[ S_{eff}^{q=3} \sim \int d^2\tau dt \left( \sum_{\alpha=0,2} |q^\alpha(\mathbf{r}, t)|^2 \right)^2 \]

(22)

leading to two doubly degenerate non-condensed modes:

\[ \omega_{\pm}^{(3)} = (\pm D_3(k) + \sqrt{D_3(k)^2 + v_3 |k|^2}/2, \]

\[ D_3(k) = -2(2\delta \mu + c_3 - v_3^2 |k|^2). \]  

(23)

Thus there are two gapped and two gapless modes with \( \omega = |k|^2 \). These two modes become gapless due to the \( O(3) \) symmetric form of \( S_{eff}^{q=3} \). For \( q > 3 \), there are in general \( 2q \) collective modes, and we have left their analysis as a subject of future study.

For experimental verification of our theory, we suggest measurement of \( n(k) \) for the bosons in the Mott phase near the transition as done earlier in ref. [3] for 2D optical lattices without the synthetic magnetic field. This distribution is predicted to display \( q \) precursor peaks. Such experiments have been carried out in the context of ultracold bosons without the synthetic magnetic fields [3] and have shown reasonable agreement with strong-coupling approach of ref. [5]. The collective modes in the superfluid phase can also be directly probed and compared to the theory by standard lattice modulation experiments [17] and response functions measurement by Bragg spectroscopy [18].

In conclusion, we have analyzed the MI-SF transition of ultracold bosons in a 2D optical lattice in the presence of a synthetic magnetic field. We have computed the momentum distribution of the bosons in the Mott phase near the MI-SF transition and have demonstrated the presence of \( q \) precursor peaks in this momentum distribution. We have provided a critical field theory for the transition and analyzed this theory to predict the superfluid ground state into which the MI-SF transition takes place. We have also calculated both the gapless and gapped collective modes of the bosons in the superfluid phase near the MI-SF transition and have provided an estimate of the masses and velocities of these modes in terms of the parameters of the Bose-Hubbard model. Finally, we have discussed possible experiments with ultracold bosonic systems which may probe our theory.

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