Phase boundary of the boson Mott insulator in a rotating optical lattice

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We consider the Bose-Hubbard model in a two-dimensional rotating optical lattice and investigate the consequences of the effective magnetic field created by rotation. Using a Gutzwiller-type variational wave function, we find an analytical expression for the Mott insulator (MI)–superfluid (SF) transition boundary in terms of the maximum eigenvalue of the Hofstadter butterfly. The dependence of phase boundary on the effective magnetic field is complex, reflecting the self-similar properties of the single particle energy spectrum. Finally, we argue that fractional quantum Hall phases exist close to the MI-SF transition boundaries, including MI states with particle densities greater than one.

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Experiments on ultracold atoms in optical lattices opened up a new avenue to study correlated quantum states [1]. The versatility of cold atom experiments hold promise for the experimental realization of many models that were first introduced for solid-state systems.

One such model is the study of particles moving in a tight binding lattice under a magnetic field. When the magnetic flux per plaquette of the lattice becomes of the order of a flux quantum hc/e, the single particle energy spectrum forms a complicated self-similar structure, known as the Hofstadter butterfly (Fig. 1) [2]. It has not been possible to reach this regime in ordinary condensed matter experiments due to the required high magnetic fields. However, the ultracold atom experiments are extremely flexible and it should be possible to create required effective magnetic fields in optical lattice experiments. A conceptually simple way of creating an effective magnetic field is to rotate the optical lattice, as demonstrated in a recent experiment [3]. Other means of creating effective magnetic fields have been discussed by a number of authors [4–11]. Although the recent demonstration of a rotating optical lattice was done for a shallow lattice, it should be possible to drive the system into the Mott insulator (MI) state by increasing the lattice depth.

In this paper, we study the Bose-Hubbard model under a magnetic field. Particularly, we consider a two-dimensional square lattice of spacing a with only nearest neighbor hopping. The magnetic field (or the effective magnetic field) strength can be expressed in terms of the dimensionless quantity ϕ, which is the magnetic flux quantum per plaquette in the lattice ($a^2H/(hc/e)$, H being the effective magnetic field). When the Landau gauge $\vec{A}=(0,Hx,0)$ is chosen, the Hamiltonian for this system can be written as

$$H = -t\sum_{\langle i,j\rangle} a_i^\dagger a_j e^{iA_{ij}} + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i \hat{n}_i, \qquad (1)$$

where a_i ($a_i^\dagger$) is the bosonic annihilation (creation) operator at site i and $\hat{n}_i=a_i^\dagger a_i$ is the number operator. The tunneling strength between nearest neighbor sites is given as t; U is the on-site interaction strength, and μ is the chemical potential. Magnetic field affects the Hamiltonian through A_{ij}, which is equal to $\pm 2\pi m\phi$, if i and j have the same x coordinate ma and is 0 otherwise, while the sign is determined by the hopping direction.

We first review some of the properties of the single particle spectrum by setting $U=0$. This problem was first discussed by Hofstadter [2]. The energy spectrum is obtained through the following difference equation (known as Harper's equation):

$$c_{m+1} + c_{m-1} + 2\cos(2\pi m\phi - k_y)c_m = \frac{E}{t}c_m,$$

where c_m are the expansion coefficients of the wave function, which has plane wave behavior along y in accordance with the translational symmetry in this direction. If ϕ is a rational number p/q, the wave function satisfies the Bloch condition $c_{m+q}=\exp(ik_xq)c_m$ as a result of the symmetry under q-site translation in the x direction. The allowed energies are then found as the eigenvalues of the $q\times q$ tridiagonal matrix as follows:

$$\mathbb{A}_q(k_x,k_y) = \begin{pmatrix} \cdot & \ddots & \cdot & \cdot & e^{-ik_xq} \\ \ddots & \ddots & 1 & \cdot & \cdot \\ \cdot & 1 & 2\cos(2\pi m\phi - k_y) & 1 & \cdot \\ \cdot & \cdot & 1 & \ddots & \ddots \\ e^{ik_xq} & \cdot & \cdot & \ddots & \cdot \end{pmatrix}. \qquad (2)$$

We call the matrix formed by setting $k_x=k_y=0$ in Eq. (2) $\mathbb{A}_q$. The maximum eigenvalue of $\mathbb{A}_q$ yields the maximum energy of the system for a given ϕ. We define this energy as $f(\phi)$, which is a continuous but not differentiable function (Fig. 1). To prove that the maximum eigenvalue is obtained from $\mathbb{A}_q$, we investigate the characteristic equation for the matrix (2), which is of the following form:

$$\left(\frac{E}{t}\right)^q + \sum_{n=0}^{q-1} a_n\left(\frac{E}{t}\right)^n - 2\cos(k_xq) - 2\cos(k_yq) = 0. \qquad (3)$$

Two pairs of (k_x,k_y), namely, (0,0) and $(\pi/q,\pi/q)$, are sufficient to determine the band edges [12]. The (0,0) pair gives a smaller value for the k_x- and k_y-dependent terms. Since the E-dependent part of Eq. (3) increases monotonically after a

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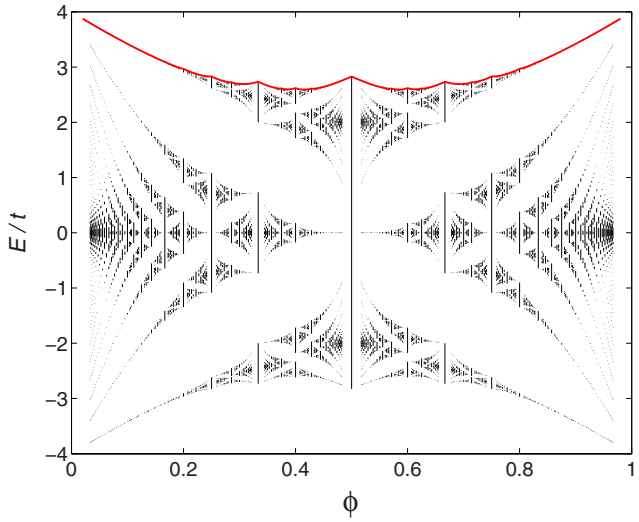

FIG. 1. (Color online) Maximum energy of the Hofstadter butterfly $f(\phi)$ for a given $\phi=p/q$. This value is calculated as the maximum eigenvalue of the matrix $\mathbb{A}_q=\mathbb{A}_q(k_x=0,k_y=0)$ [Eq. (2)].

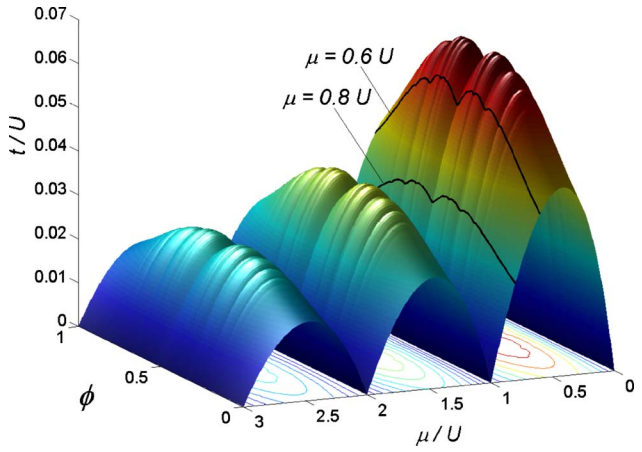

FIG. 2. (Color online) The boundary of the Mott insulator phase for the first three Mott lobes. The figure is periodic in ϕ. Magnetic field increases the critical value for t/U, as expected; however, this increase is not monotonic. Transition boundary for two different values of μ/U are marked to display the complex structure of the surface.

sufficiently large E, the greatest root is always obtained from the (0,0) pair.

We now turn to the interacting case with the dimensionless Hamiltonian as follows:

$$\tilde{H} = -\tilde{t}\sum_{\langle i,j\rangle} a_i^\dagger a_j e^{iA_{ij}} + \frac{1}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \tilde{\mu}\sum_i \hat{n}_i, \tag{4}$$

where $\tilde{t}=t/U$ and $\tilde{\mu}=\mu/U$ are the scaled hopping strength and chemical potential.

When the hopping term is dominant $\tilde{t}\gg 1$, one expects the system to be in a SF state, while in the opposite limit of strong interactions $\tilde{t}\ll 1$, the system should go into the MI state. In this paper, we investigate the transition boundary between these two phases, and how this boundary is affected by the external magnetic field. The effect of the magnetic field on the transition boundary has been previously explored by strong coupling expansion for small magnetic fields by Niemeyer *et al.* [13], and numerically within mean-field theory by Oktel *et al.* [14]. Here we use a variational approach to provide an analytical expression for the transition boundary.

We use a site-dependent Gutzwiller ansatz to describe the system [15]. For the Bose-Hubbard model without magnetic field, this ansatz (and equivalent mean-field theory [16–18]) gives an accurate description of the phase diagram. We introduce the variational wave function at each site l,

$$|G\rangle_l = \Delta_l|n_0-1\rangle_l + |n_0\rangle_l + \Delta_l'|n_0+1\rangle_l. \tag{5}$$

Since we investigate the behavior in the vicinity of the transition region, we consider small variations around the perfect MI state with exactly n_0 particles per site, allowing for only one less or one more particle in a site. The variational parameters Δ_l and Δ_l' are assumed to be real, as complex Δ values can only increase the energy of the variational state. Total wave function is the direct product of these site wave functions $|\Psi\rangle=\Pi_i^N|G\rangle_i$. Within the selected gauge, the magnetic Hamiltonian has translational invariance in the y direction. The translational invariance in the x direction is broken by the magnetic field, but can be restored to a certain degree if the flux per plaquette is a rational number. Thus, taking $\phi=p/q$, where p and q are relatively prime integers, the Hamiltonian is invariant under translation by q sites in the x direction. This periodicity simplifies the calculation of the expectation value of the energy when we work with a supercell of $1\times q$ sites. Total wave function for such a supercell is $|\Psi\rangle_s=\Pi_{l=0}^{q-1}|G\rangle_l$. The expected value of the energy can then be written as follows:

$$\frac{\langle\Psi|\tilde{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = N_s\frac{{}_s\langle\Psi|\tilde{H}|\Psi\rangle_s}{{}_s\langle\Psi|\Psi\rangle_s} \equiv N_s\epsilon, \tag{6}$$

where N_s is the number of supercells.

Keeping terms up to second order in the variational parameters Δ, the energy of a supercell is calculated as

$$\begin{aligned}\varepsilon = \sum_{l=0}^{q-1}\Bigg(&-2\tilde{t}\Big\{n_0\Delta_l\Delta_{l+1} + \sqrt{n_0(n_0+1)}\Delta_l\Delta_{l+1}' \\ &+ \sqrt{n_0(n_0+1)}\Delta_{l+1}\Delta_l' + (n_0+1)\Delta_l'\Delta_{l+1}' \\ &+ \cos\left(2\pi\frac{p}{q}l\right)[n_0\Delta_l^2 + 2\sqrt{n_0(n_0+1)}\Delta_l\Delta_l' \\ &+ (n_0+1)(\Delta_l')^2]\Big\} + \frac{1}{2}[2(1-n_0)\Delta_l^2 + 2n_0(\Delta_l')^2 \\ &+ n_0(n_0-1)] + \tilde{\mu}[\Delta_l^2 - (\Delta_l')^2 - n_0]\Bigg).\end{aligned} \tag{7}$$

If the system favors to be in the Mott insulator state, the total energy of the system should be a minimum where all the variational parameters vanish. Thus, we can find the phase boundary as the point where the total energy ceases to be a local minimum in Δ. As a result, we demand that the matrix

composed of the second derivatives of ε with respect to the parameters $(\partial^2\varepsilon/\partial\Delta_i\partial\Delta_j, \partial^2\varepsilon/\partial\Delta_i\partial\Delta_j', \partial^2\varepsilon/\partial\Delta_i'\partial\Delta_j')$ be positive definite, i.e., all eigenvalues be positive. This matrix can be written compactly as

$$\mathbb{F} = -2\tilde{t}\begin{pmatrix} n_0\mathbb{A}_q & \sqrt{n_0(n_0+1)}\mathbb{A}_q \\ \sqrt{n_0(n_0+1)}\mathbb{A}_q & (n_0+1)\mathbb{A}_q \end{pmatrix} + \begin{pmatrix} 2(1-n_0+\tilde{\mu})\mathbb{I}_q & 0 \\ 0 & 2(n_0-\tilde{\mu})\mathbb{I}_q \end{pmatrix},$$

where $\mathbb{I}_q$ is the $q\times q$ identity matrix, and $\mathbb{A}_q$ was introduced before [Eq. (2)].

If we denote the eigenvalues and eigenvectors of $\mathbb{A}_q$ by λ_ν and $\vec{\nu}$, and those of $\mathbb{F}$ by λ_u and $\vec{u}$, all λ_u can be expressed in terms of λ_ν by taking

$$\vec{u} = \begin{pmatrix} a\vec{\nu} \\ b\vec{\nu} \end{pmatrix},$$

due to the special block form of $\mathbb{F}$. Then λ_u are obtained as

$$\lambda_u^{\mp} = 1 - (1+2n_0)\tilde{t}\lambda_\nu \mp \sqrt{[(1+2n_0)\tilde{t}\lambda_\nu - 1]^2 - 4\{(n_0-\tilde{\mu})[1-(n_0-\tilde{\mu})] - \tilde{t}(1+\tilde{\mu})\lambda_\nu\}}.$$

The positive definiteness of $\mathbb{F}$ leads us to take λ_u^- and set it to zero in order to determine the critical $\tilde{t}$ value above which the perfect insulator state is destroyed. We find the boundary of the n_0th Mott lobe to be

$$\tilde{t}_c = \frac{(n_0-\tilde{\mu})[1-(n_0-\tilde{\mu})]}{(1+\tilde{\mu})f(\phi)}, \tag{8}$$

where $n_0-1\leq\tilde{\mu}\leq n_0$. This boundary is plotted in Fig. 2 for the first three Mott lobes. At $\phi=0$, this formula reproduces the critical $\tilde{t}$ value found in [16,17]. Increasing the magnetic field increases the critical hopping strength $\tilde{t}_c$, however, this increase is not monotonic. The complicated structure of the single particle problem is reflected in the transition boundary. Equation (8) is in excellent agreement with the numerical mean-field work [14].

We can comment on the accuracy of our variational approach. Our result is exact within mean-field theory. At zero magnetic field the mean-field result for the transition boundary is close to accurate Monte Carlo calculations [19], but it is not guaranteed that the mean-field description of the system would be valid under magnetic field. Our variational wave function (and mean-field theory) disregards the correlations between fluctuations above the insulating state. Such correlations would be expected to wash out the fine structure of the transition boundary (Fig. 2). Nevertheless, one can expect a number of features of the mean-field boundary to survive for the real system. The linear increase of the transition point for small magnetic fields, periodicity of the system with ϕ, and the central dip near $\phi=0.5$ should be qualitatively correct.

There is, however, one important way that the fluctuations around the Mott insulating state can become correlated. The Hamiltonian (4) supports bosonic fractional quantum Hall (FQH) states as discussed in a number of recent papers [7,20,21]. So far, such FQH states have been assumed to appear only in the region of low density where the number of particles per site is less than one. Here, we argue that states similar to bosonic FQH states should be present near the MI boundaries, even at higher densities.

It is instructive to think about the behavior of the Hamiltonian for constant particle density by disregarding the last term. Let us assume that the particle density is equal to $n=n_0+\epsilon$, where n_0 is an integer and $\epsilon\ll 1$ is the decimal part of the density. With such an incommensurate particle number, the system never goes into the MI state, but will always have a superfluid density. The chemical potential for this state, plotted on the $\tilde{\mu},\tilde{t}$ plane, traces the outline of the Mott lobe as the interaction is increased (Fig. 3). However, if we think of the same system under a magnetic field that is commensurate with the excess particle density, another possibility presents itself. Specifically, considering a magnetic field so that $\phi=2\epsilon$, it is possible for n_0 particles to form a MI state that is coexisting with a $\nu=1/2$ bosonic Laughlin state of the remaining ϵ particles. At high enough interaction, such a state would be preferable to a superfluid state as it avoids any interaction between the "excess" particles. The wave function of such a state can be obtained by symmetrizing the product of the Mott insulator state for n_0 bosons with the $\nu=1/2$ bosonic Laughlin state for ϵ particles. In general, separating the many particle wave function into two parts and arguing that the overall properties can be deduced by thinking about the individual parts is not correct, as symmetrization may change the character of both parts considerably. In this case, however, we can safely regard the excess particles as forming a correlated state above the Mott insulator, due to the full translational invariance of the MI state. One can write down an effective Hamiltonian for the excess particles. To the zeroth order, the change in the effective Hamiltonian would be just to replace t by $(n_0+1)t$, due to bosonic enhancement of the hopping. There will be higher order corrections to t and new noncontact interaction terms between the excess particles due to fluctuations in the MI state. Such terms will be of higher order in (t/U), and can be neglected in the strongly interacting limit. One can also argue that as

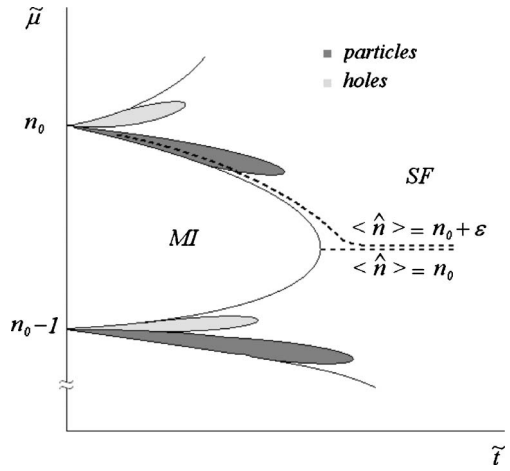

FIG. 3. Schematic phase diagram near the n_0th Mott lobe. Dotted lines show the chemical potential as a function of hopping strength for systems with constant density $\langle\hat{n}\rangle=n_0$ and $\langle\hat{n}\rangle=n_0+\varepsilon$. FQH phases of "excess" particles or holes are shown as the shaded regions.

both the MI state and the bosonic Laughlin state are gapped, it would not be energetically favorable to exchange particles between the two parts of the wave function. Similarly, one can argue that the overall state would be gapped in the strongly interacting limit.

Treating such a state as a variational state, the energy difference from the MI state can be written as

$$\Delta E = [Un_0 - \mu - t(n_0+1)f(\phi)]\epsilon. \tag{9}$$

To first order in t/U, the term in parentheses is the energy needed to put one extra particle onto the Mott insulator. Thus, when it is favorable to put one extra particle onto the Mott state, it would be favorable to put more particles (up to ϵ per site) and organize them into a FQH state. One can then expect the correlated state to exist within a band above the MI lobe (see Fig. 3). The same argument can be advanced for holes in a MI state, creating a FQH of holes below the Mott insulator. Detailed properties of these correlated states, as well as other correlated states near the transition boundary will be investigated elsewhere [22].

The phase diagram in Fig. 3 has important implications for the optical lattice experiments. Experimentally an overall confining potential is always present, and the phase diagram of the homogeneous system is valid only in the local density approximation. Thus a trapped system samples a range of local chemical potentials from the phase diagram. It is this sampling which creates the "wedding cake" structure of alternating SF-MI layers in an optical lattice with an external potential. One can observe from Fig. 3 that, a rotating optical lattice in an external confining potential still shows the wedding cake structure; however, the density profile has extra steps corresponding to FQH states.

In conclusion, we studied the phase boundary of the MI state of bosons in a rotating optical lattice. Using a Gutzwiller ansatz, we gave an analytical expression for the phase boundary in terms of the maximum energy of the Hofstadter butterfly. We finally argued that analogs of FQH states will be found close to the MI-SF transition boundary including MI states with particle densities greater than one.

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