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Bose–Hubbard phase transition with two- and three-body interaction in a magnetic field

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ABSTRACT

Phase boundaries of classical and quantum phase transitions of two-dimensional Bose–Hubbard model with two- and three-body on-site interactions in a magnetic field are obtained analytically in a unified theoretical frame. All results illustrate that the introduction of magnetic field enhances the stability of normal state and Mott insulator.

1. Introduction

Bose–Hubbard model of interacting bosons on a lattice has been used to describe superfluid-Mott insulator (MI) phase transition in a variety of systems at zero temperature, e.g., Josephson arrays and granular superconductors [1]. The recent suggestion to experimentally observe this transition in a system of cold bosonic atoms in an optical lattice [2] and its successful experimental demonstration [3] have aroused much theoretical [4–6] and experimental [7,8] interests in this model. However in original Bose–Hubbard model interactions among three and more bosons are completely neglected, and the system is merely controlled by the two-body interaction and tunneling effect which allow bosons to hop around within the optical lattice. This kind of simple description for the Hamiltonian is the reflection of pairing theory in condensed matter physics that particles interactions can be approximated as a summation of pairwise events. Although pairing theory plays an important role historically and also contains many ideas which are qualitatively correct, the plethora of exotic quantum phases, such as string nets [9], are often associated with ground states of Hamiltonians with three or more body terms.

In fact, the research of three-body interaction originated from accurate calculation of ground state energy of boson system in 1959 [10]. Following the achievement of Bose–Einstein-Condensate in 1995 determinations on detailed properties of three-body interaction were revived [11,12], furthermore Büchler et al. [13] have suggested that polar molecules driven by microwave fields give naturally rise to strong three-body interaction and derived the complicated phase diagram of one-dimensional Bose–Hubbard model with dominant three-body interaction.

Recently Chen et al. [14] have studied quantum phase transition between superfluid state and Mott insulator based on Bose–Hubbard model with two- and three-body on-site interactions at the mean field level and found some interesting phenomena such as the rotation of phase boundary around a fixed point and extended areas of Mott insulator. To the best of our knowledge an unstudied problem is that of the Bose–Hubbard Hamiltonian under a magnetic field. As is known to all that bosons used in cold gas experiments are uncharged and would not be directly affected by an external magnetic field. However, recent studies have shown in detail that effective magnetic field, even non-Abelian magnetic field, can be generated for neutral atoms generally by two methods. Perhaps the simplest and most common method is rotating the whole system, and canceling the centrifugal force of the rotation by an external quadratic trap [15], while the other one [16] is by means of laser methods employing dark state. This method is based on the fact that the adiabatic motion of a λ-type three-level atom creates a nondegenerate dark state in the presence of external laser fields. In addition there are also other methods to create artificial magnetic field such as Laser-assisted tunneling and lattice tilting [17], BEC immersion [18] and two-photon dressing by laser fields [19]. Irrespectively of which method we adopt, the fundamental effect on the system is qualitatively similar.

In this Letter, we are interested in classical and quantum phase transitions of Bose–Hubbard model with two- and three-body

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on-site interactions under a magnetic field and assume a two-dimensional square lattice in the XY plane, under a magnetic field in the Z direction. Two-dimensional Bose–Hubbard model is easily achieved by imposing strong laser to suppress the tunneling effect along Z axis. At zero temperature the phase transition, which are driven by quantum fluctuation and called quantum phase transition, happens between superfluid phase and MI, while at finite temperature MI is replaced by normal state which possesses finite compressibility so the phase transition happens between superfluid phase and normal state, which are driven by the competition between energy and entropy and called classical phase transition. Here we do not include the crossover from MI to normal state at finite temperature since there is not a conventional definition for this crossover as far as what we know is concerned. In Section 2, an effective single-site Hamiltonian is written out by decoupling hopping term, then we point out the similarity between this reduced Hamiltonian and that of Bose–Hubbard model in an one-dimensional superlattice for the purpose of finding the solution. In Section 3, we analytically derive the phase boundaries of classical and quantum phase transition under a unified frame by analyzing the stability of normal state, at the same time numerical results with and without the magnetic field are also shown. A brief conclusion is given in Section 4.

2. Theory

The Hamiltonian of Bose–Hubbard model with on-site two-body interaction in a magnetic field is derived in details in [20]. The inclusion of on-site three-body interaction is very direct, so the Hamiltonian in this Letter is

$$H = -t\sum_{\langle ij\rangle}\exp\left[i2\pi\phi\int_{\vec{r}_j}^{\vec{r}_i} x\,dy\right]b_i^\dagger b_j + \frac{U}{2}\sum_i n_i(n_i-1) + \frac{W}{6}\sum_i n_i(n_i-1)(n_i-2) - \mu\sum_i n_i \tag{1}$$

where the summation in the first term is done for the nearest neighbors only and $b_i^\dagger$ (b_i) is the bosonic creation (annihilation) operator with $n_i = b_i^\dagger b_i$ the particle number operator for bosons at the lattice site i. The parameter t is the hopping term and U, W are two- and three-body repulsive interaction strength among bosons. The last term involving the chemical potential μ is added because it is very convenient to work in the grand canonical ensemble. All the coordinates $\vec{r}_i$, x, y are scaled by the lattice constant a hence are dimensionless. $\phi = Ba^2/(hc/e)$ represents the number of magnetic flux quanta penetrating the unit cell with B being effective magnetic field and $\phi_0 = hc/e$ magnetic flux quanta. The presence of the effective magnetic field introduces factor $\exp[i2\pi\phi\int_{\vec{r}_j}^{\vec{r}_i} x\,dy]$, called Peierls phase factor which completely absorbs the effect of the magnetic field, to modify hopping term but keeps interaction terms invariant. Thus in contrast to nonmagnetic solution [14] we naturally expect a modified phase boundary in view of the fact that superfluid-Mott insulator phase transition comes from the competition between hopping term and on-site interaction strength. In fact the Hamiltonian (1) is an expression under Landau gauge in which hopping along the Y axis only achieves the Peierls phase factor, and we can also alter the Peierls phase factor by transforming to other gauge.

$U = W = 0$ corresponds to noninteracting bosons. In this case the energy spectrum of Hamiltonian, denoted by Hofstadter butterfly [21], shows a self-similar fractal structure on the energy-magnetic flux plane. The experimental observation of this energy spectrum is very difficult due to weak magnetic field and small area of lattice cell. As suggested by Jaksch and Zoller [17], it is promising to observe Hofstadter butterfly in ultracold atom gas in the light of their highly controllability and operability. Below we will regard the Hamiltonian (1) as our starting point to study its zero and finite temperature phase diagram by Gutzwiller approximation, and will find that the Hofstadter butterfly have an important effect on phase boundary.

The Gutzwiller approach is a self-consistent mean-field method and equivalent to the decoupling approximation [22,23] to the hopping term

$$b_i^\dagger b_j = \langle b_i^\dagger\rangle b_j + b_i^\dagger\langle b_j\rangle - \langle b_i^\dagger\rangle\langle b_j\rangle = \alpha_i b_j + b_i^\dagger\alpha_j - \alpha_i\alpha_j \tag{2}$$

where $\alpha_i = \alpha_i^*$ is superfluid order parameter which distinguishes the superfluid phase from normal state. If magnetic field vanishes, the whole system is uniform and order parameter is also site-independent. But we cannot suppose this when the magnetic field appears. After this decoupling, the system is describable in terms of a single-site Hamiltonian

$$H_{nm} = -t\big[b_{nm}^\dagger\big(\alpha_{(n+1)m} + \alpha_{(n-1)m} + e^{-i2\pi n\phi}\alpha_{n(m+1)} + e^{i2\pi n\phi}\alpha_{n(m-1)}\big) + \text{H.C.}\big] + \frac{U}{2}n_{nm}(n_{nm}-1) + \frac{W}{6}n_{nm}(n_{nm}-1)(n_{nm}-2) - \mu n_{nm} \tag{3}$$

where we label the site of lattice i by two ordered integers (n, m), the first integer along the X axis and the second along the Y axis. The Hamiltonian (3) has two striking characteristics. On one hand its independence of Y component implies that system is translational invariant along Y axis and we can suppose that order parameter $\alpha_{nm} = \alpha_n$ is independent of Y component. On the other hand although it depends on X component, for rational $\phi = p/q$ (p, q have no common factor) q-site translational symmetry along X axis is recovered and the order parameters have periodicity $\alpha_n = \alpha_{n+q}$. The statement above drops a hint that our calculations will be carried out on a $q\times 1$ supercell with periodic boundary conditions [24]. So the Hamiltonian is further reduced into

$$H_n = -t\big[b_n^\dagger(\alpha_{n+1} + \alpha_{n-1} + 2\alpha_n\cos 2\pi n\phi) + \text{H.C.}\big] + \frac{U}{2}n_n(n_n-1) + \frac{W}{6}n_n(n_n-1)(n_n-2) - \mu n_n \tag{4}$$

with n being integer from 1 to q. In addition, the Hamiltonian is periodic as the function of magnetic field $H_n(\phi) = H_n(\phi + K)$ with K being a random integer so that we only need consider $\phi\in[0,1)$. Note also that in (3) and (4) we have neglected a constant term which does not influence our result.

Now in order to find out solution for the reduced Hamiltonian (4) more quickly, we compare the Hamiltonian (1) with that of one-dimensional superlattice without magnetic field where there are some nonequivalent atom sites in a single cell [25]. Easily found that under the same Gutzwiller approximation two Hamiltonians are almost the same, and superlattice cell plays the same role as $q\times 1$ supercell we mentioned above if there are q atom sites in superlattice cell. In view of this similarity the analytical solution of reduced Hamiltonian (4) is viable.

The self-consistency of Gutzwiller method must be implemented by the condition

$$\alpha_n = \frac{1}{Z_n}\text{Tr}\big(b_n e^{-\beta H_n}\big) = \frac{1}{Z_n}\text{Tr}\big(b_n^\dagger e^{-\beta H_n}\big) \tag{5}$$

with $\beta = 1/(K_B T)$ and partition function $Z_n = \text{Tr}\exp(-\beta H_n)$. Introducing the notation $\gamma_n = t\alpha_n$, self-consistent condition can be