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Quantum Phase Transition of the Bosonic Atoms near the Feshbach Resonance in an Optical Lattice *

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The quantum phase transition from the Mott insulator to the superfluid phases of the bosonic atoms trapped in an optical lattice, in which the on-site interaction can be tuned by a Feshbach resonance, is investigated by a variational approach within mean-field theory. We derive an extended Bose–Hubbard model to describe this ultracold atomic system. By theoretical calculation and analysis, the phase diagram is shown clearly, and we find an exciting and novel phenomenon that is the appearance of the Mott insulator-sea (MI-sea). Meanwhile, the experimental feasibility of observing the MI-sea is discussed by analyzing the published data related to the Fashbach resonance at present. Finally, the potential application of the MI-sea for quantum information processing and quantum computation is also discussed in detail.

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The Bose–Hubbard model (BHM) originating from the Hubbard model in solid state physics[1,2] has been widely studied theoretically[3–5] and experimentally[6–9] in recent years, due to the natural advantage that the system character can be observed with a high accuracy and the system parameters including the optical lattice depth, and the on-site interaction strength can be controlled accurately,[10] it describes the physics of interacting bosonic atoms in an optical lattice. Moreover, the BHM has been extended to other relative physics systems such as the Fermion–Hubbard model,[11–13] the Bose–Fermi–Hubbard model[14–16] and the Jaynes–Cummings–Hubbard model,[17–21] these models provide optimum candidates for quantum simulation with ultracold atoms, which can be used to research problems in various fields including atomic physics, condensed-matter physics, cosmology and so on.[22]

The optical lattice and the Feshbach resonance are two major tools for studying the physics of the ultracold atoms represented by BHM,[10,23,24] because the optical lattice provides a periodic light potential to ultracold atoms and the Feshbach resonance can be used to tune the interaction between the ultracold atoms in a large range.

The Hamiltonian for the standard BHM can be written as[4,10,25]

$$\mathcal{H} = -t\sum_{\langle ij\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + U'\sum_i n_i(n_i-1) - \mu\sum_i n_i, \tag{1}$$

where $a_i^\dagger$ and a_i are the annihilation and creation operators on the lattice site i, the operators $n_i = a_i^\dagger a_i$ denote the number of the bosonic atoms at site i, $\langle ij\rangle$ denotes the summating only for the nearest neighbors. The parameter[10,26] $t \simeq (4/\sqrt{\pi})E_r(V_0/E_r)^{3/4}\exp(-2\sqrt{V_0/E_r})$ is the hopping matrix element between adjacent sites with a recoil energy E_r and an optical lattice depth V_0, $U' = \sqrt{8/\pi}kaE_r(V_0/E_r)^{3/4}$ corresponds to the on-site interaction of two atoms in the same lattice site,[10,26] $k = 2\pi/\lambda$ is the optical lattice wave vector and λ is the laser wave length, a is the atoms scattering length, and μ is the chemical potential.

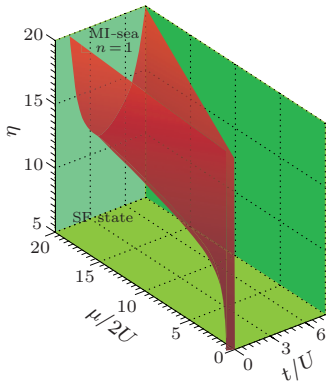


Fig. 1. (Color online) Phase diagram of the extended Bose–Hubbard model, in which ultracold bosonic atoms are trapped in an optical lattices and subject to a Feshbach resonance, for the MI ($n = 1$) state in the case of continuous varying the value of η. The red curved surfaces describe the phase boundary between the Mott insulator and the Superfluid states when each lattice site has only one bosonic atom. The existing MI-sea is a key and symbolic feature compare with general standard Bose–Hubbard model.

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As is well known,[3–5] this BHM system will be in the Mott-insulator state when the on-site interaction term is too large, or in the superfluid (SF) state when the interaction term is too small, compared with the hopping term. The phase transition from SF to MI phases will occur by varying the ratio between the interaction and the hopping terms. In previous works,[6–9] however, the parameters t and U can be only tuned by varying the lattice depth V_0. This gives us a limitation for varying individually the hopping and on-site interaction terms. In addition, the Feshbach resonance has been mainly used to investigate the ultracold Fermions[27,28] and Bose–Fermion mixture gases,[10,29–31] namely the role of the Feshbach resonance for the quantum phase transition of bosonic atoms trapped in an optical lattice is not appreciated until now.

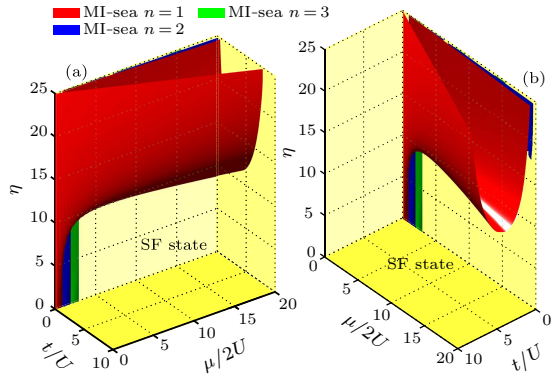


Fig. 2. (Color online) Phase diagram of this extended Bose–Hubbard model for the MI ($n = 1, 2, 3$) states from different points of view. The red, blue and green curved surfaces describe the phase boundaries between the Mott insulator and the Superfluid states when each lattice site has one, two and three bosonic atoms, respectively.

In this Letter, we confront and solve these problems by considering an extended BHM, in which the ultracold bosonic atoms are trapped in an optical lattice and are subject to a Feshbach resonance. In this case, the atoms scattering length a [10,24] as a function of the applied magnetic field B can be written as $a(B) = a_{bg}[1 - \Delta B/(B - B_0)]$, where a_{bg} is the off-resonant background scattering length in the absence of the coupling to the closed channel, ΔB and B_0 are the width and position of the resonance. By further calculation, we can obtain the formula $U' = U + t\eta$, where $U = \sqrt{8/\pi}ka_{bg}E_r(V_0/E_r)^{3/4}$ indicates the on-site interaction induced by the background scattering length.

The key parameter for this extended BHM,

$$\eta = \frac{ka_{bg}}{\sqrt{2}} \exp\left(2\sqrt{\frac{V_0}{E_r}}\right) \frac{\Delta B}{B_0 - B}, \tag{2}$$

can be tuned by varying the applied magnetic field.

Thus, the Hamiltonian described this extended Bose–Hubbard system can be written as

$$\mathcal{H} = -t\sum_{\langle ij\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + (U + t\eta)\sum_i n_i(n_i - 1) - \mu\sum_i n_i. \tag{3}$$

We begin to calculate the Hamiltonian by variational approach, and use the decoupling formula[32]

$$a_i^\dagger a_j = \langle a_i^\dagger\rangle a_j + a_i^\dagger\langle a_j\rangle - \langle a_i^\dagger\rangle\langle a_j\rangle, \tag{4}$$

where $\langle a_j\rangle$ is the average value of the operator a_j. It expresses the order parameter Ψ_j of the system, which indicates the quantum phase transition. In the MI state, the particle number on each lattice site is definite, and the order parameter is equal to zero. On the other hand, if the system is in the SF state, the order parameter has a nonzero value due to the large quantum fluctuation of the particle number in the optical lattice. In addition, the local density of the bosonic atoms in the condensate state can be described by $|\Psi_j|^2$.

After using the above formula, the Hamiltonian given in Eq. (3) can be turned into a sum of the following single-site terms:

$$\mathcal{H}_i^{MF} = -t(\Psi_{i+1}a_i^\dagger + \Psi_{i-1}^* a_i + \text{H.c.}) + (U + t\eta)n_i(n_i - 1) - \mu n_i + C_i, \tag{5}$$

where C_i is a constant energy term.

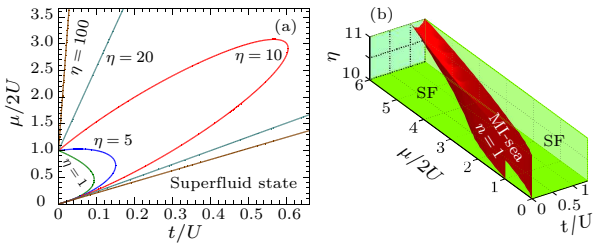


Fig. 3. (Color online) Development and formation of the MI-sea in this extended Bose–Hubbard model when each lattice site has only one bosonic atom.

To describe this ultracold atoms system, we use a Gutzwiller ansatz,[33,34] which can accurately express the phase diagram for a standard BHM. Then, the total variational wave function of the system can be described by a direct product of all-site wave function $|\Phi\rangle = \prod_i |\phi\rangle_i$. We consider a small variations around the perfect MI state with exactly n ultracold atoms per site, and introduce the single-site wave function

$$|\phi\rangle_i = \alpha_i|n-1\rangle_i + \sqrt{1 - {\alpha_i}^2 - {\beta_i}^2}|n\rangle_i + \beta_i|n+1\rangle_i, \tag{6}$$

where α_i and β_i are the probability amplitude for the occurring small variations, $|n\rangle$ denotes the state with n bosonic atoms.

The expected value of the energy for this system can be described by

$$\frac{\langle\Phi|\mathcal{H}|\Phi\rangle}{\langle\Phi|\Phi\rangle} = N\mathscr{E}, \tag{7}$$

and by minimuming the variational parameters we can obtain the phase boundary as follows:

$$\frac{t}{U} = \frac{[(1+\frac{t}{U}\eta)n - \frac{\mu}{2U}][(1+\frac{t}{U}\eta)(1-n) + \frac{\mu}{2U}]}{2(1+\frac{t}{U}\eta+\frac{\mu}{2U})}. \tag{8}$$

The corresponding three-dimensional phase diagrams are shown in Figs. 1 and 2.

The best exciting and novel discovery (see Fig. 1) in this phase diagram is the appearance of a space, in which the MI states are permeated if the value of η is large enough, we call it an MI-sea that is of inexistence for a standard BHM without an applied magnetic field. When η is very small, the red curved surface, which describes the phase boundary between the SF and MI states for $n = 1$, together with the $\eta-\mu/2U$ plane constitute a semi-closed space that is full of the MI states. Under this condition, the influence induced by η in the phase diagram is not evident. On the contrary, if η is very large, the space will be open and it will be like the unbounded ocean, just this sea floats on the SF states. This reflects the role of η, and is also the key in this study. Meanwhile, we also find that for $n = 2$ and $n = 3$ (see Fig. 2), the MI-sea also exists in the phase diagram for this extended BHM. Moreover, each MI-sea has an independent space and not overlapping for different MI-sea, just different MI-seas have different shapes, which become more and more apparent with the increase of particle numbers in the MI state for each lattice.

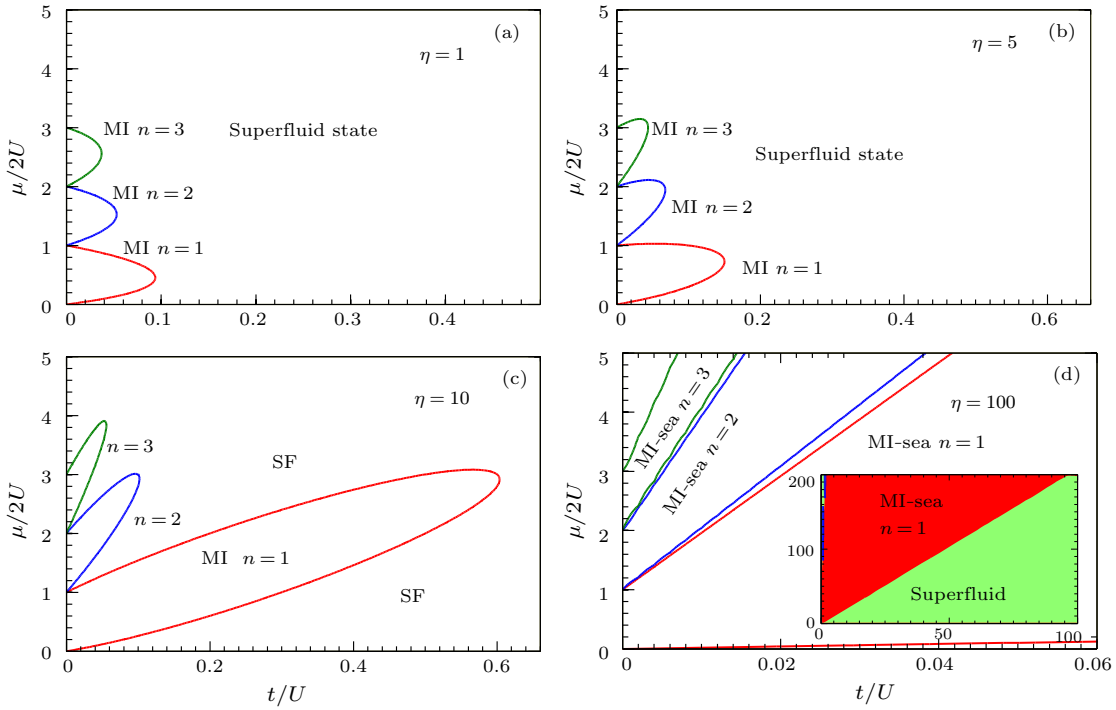


Fig. 4. (Color online) Phase diagram of the extended Bose–Hubbard model for the first three MI-sea. The red, blue and green curves describe the phase boundaries between the Mott insulator and the Superfluid states for $n = 1, 2, 3$, respectively. (a) The first three Mott lobes when $\eta = 1$, which are almost the same as the phase diagram of a standard Bose–Hubbard model. The inset in (d) describes the space distribution of the Mott and superfluid states.

Here we emphasis the range of values of η by analyzing the experimental data, and show two key points. The first is that η can be significantly small, while it cannot be zero. For example, we use the data in Refs. [24,35], $B_0 = 406.2G$, $\Delta B = 4 \times 10^{-4}$ G, $a_{bg} = 100a_0$, where a_0 is the Bohr radius, if we take $\lambda = 700$ nm, $V_0 = 16E_r$ and $B = 366.2$ G, by calculation, we can obtain $\eta = 1.8 \times 10^{-5}$. In this case, the phase diagram has no essential difference with a standard BHM given in Refs. [4,10,25], due to the fact that the value of η is far less than the value of η for obvious appearing MI-sea. The second that observing the MI-sea in experiment is realizable. As an example, we consider the experimental data in Ref. [24], $B_0 = 547$ G, $\Delta B = 7.5$ G, $a_{bg} = 2500a_0$, and we take $\lambda = 700$ nm, $V_0 = 16E_r$, for different values of B, the calculation results are $\eta_{B=478.1\,\mathrm{G}} = 5$, $\eta_{B=512.6\,\mathrm{G}} = 10$. In fact, the value of η will increase during the value of B closing to B_0. This gives us a simple and controlled experimental condition for realizing the quantum phase transition and for observing the absence of the MI-sea in this extended BHM.

The development and formation of the MI-sea has been shown in Fig. 3 for $n = 1$ and in Fig. 4 for the

first three MI-sea. When the value of η is small, the shape of the Mott lobe is the same as a standard BHM. However, as the value of η increases, the difference becomes very apparent, reflecting that the sharp peak of the Mott lobe starts graduate moving along $\mu/2U$ and t/U directions, and the space possessed by MI state will increase, but the intersecting point of the Mott lobe and the $\mu/2U$ axis will hold the line in the case of two dimensions, for three-dimensional case, the interacting lines of the boundary and the η-$\mu/2U$ plane will be always perpendicular to the t/U-$\mu/2U$ plane. A likely explanation is that, as the value of η increases, the Mott state in the semi-closed space breaks the siege by boundary and burst forth to space original belongs to superfluid state, to form the MI-sea. When the value of η is large enough, the MI state will take up about half space in the two-dimensional phase diagram, and almost the same as the superfluid state.

We now point out the potential application of this MI-sea for quantum information processing and quantum computation. The scheme of the distributed quantum computation based on small quantum registers has been presented by Jiang *et al.* in 2007,[36] and the realization approach of the register based on the individual alkaline-earth-metal atoms trapped in an optical lattice has also been proposed by Gorshkov *et al.* in 2009,[37] in which an assumed condition for the realization of the interregister gate is that atoms are prepared in an MI state in an optical lattice. Thus the stability and the capacity of resisting disturbance of the MI state is a key experimental condition for the research of the quantum computation. For this problem, the existence of the MI-sea provides a nature experimental system. As a example, for $n = 1$, so long as we adjust the value of η, the system will be in the MI state without reference to the varying of t/U and $\mu/2U$. In fact, this novel and practical platform can be used to research the properties of the MI state and quantum simulation and so on.

In conclusion, we have studied the phase boundary between the MI and the SF states of ultracold bosonic atoms trapped in an optical lattice and subject to a Feshbach resonance. Using the variational approach within the mean-field theory, we give an analytical expression for the phase boundary from the SF to the MI state with a tunable parameter η, which reflects the role of the Feshbach resonance. The phase diagram of this extended BHM has also been shown in the form of three and two dimensions, the best exciting and novel discovery is the existence of the MI-sea. We also discuss the feasibility in experimental by analyzed experimental data. Furthermore, the properties, development and formation of the MI-sea has been described in detail. We finally argue the potential application of the MI-sea in quantum information processing, quantum computation and other fields.

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