Ground-state competition of two-component bosons in an optical lattice near a Feshbach resonance

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We investigate the ground-state properties of an equal mixture of two species of bosons in its Mott-insulator phase at a filling factor of two per site. We identify one type of spin triplet-singlet transition through the competition of the ground state. When the on-site interaction is weak ($U<U_c$) the two particles prefer to stay in the lowest band and with weak tunneling between neighboring sites the system is mapped into an effective spin-1 ferromagnetic exchange Hamiltonian. When the interaction is tuned by a Feshbach resonance to be large enough ($U>U_c$), the higher band will be populated. Due to the orbital coupling term S^+S^- in the Hamiltonian, the two atoms in different orbits on a site would form an on-site singlet. For a non-SU(2)-symmetric model, easy-axis or easy-plane ferromagnetic spin exchange models may be realized, corresponding to phase separation or counterflow superfluidity, respectively.

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The study of quantum phase transitions in optical lattices has made great progress both theoretically and experimentally [1,2] and has become one of the focus issues of current interest in the exploration of rich physics in ultracold atomic systems. Jaksch *et al.* predicted that the dynamics of a single-component Bose gas loaded into the lowest band of an optical lattice is well described by the Bose-Hubbard model [1] and Greiner *et al.* experimentally confirmed that the phase transition from superfluid phase to Mott insulator could be realized by suppressing tunneling between neighboring sites [2]. For single-component bosons without internal degrees of freedom, the superfluid-insulator transition in a periodic lattice has been extensively studied by various methods [1,3,4]. When the spinless bosons are in the Mott phase, the on-site fluctuation of particle numbers is suppressed [4]. Many studies have shown that multicomponent bosonic or fermionic gases in optical lattices exhibit much richer phase diagrams [5–10]. An intriguing feature of the multicomponent Bose systems is the structure of their internal "spin" degree of freedom. The recent formation of bound repulsive atom pairs in an optical lattice even exemplifies stable states without any analog in traditional condensed matter physics [11].

So far, a number of schemes have been proposed to derive an effective Hamiltonian to describe the spin-related dynamics for the multicomponent system in the Mott-insulator phase [7,8]. Most of the schemes ignore the existence of the upper bands and take the single-band approximation, which is reasonable when the on-site interaction is much smaller than the energy gap between the first band and the second one. The situation may change dramatically if the scattering strength of the atoms is greatly enhanced by the Feshbach resonance so that the on-site interaction exceeds the band gap. Recently, Köhl *et al.* have studied a fermionic mixture of two hyperfine states of ^{40}K, in a three-dimensional optical lattice and accessed the strongly interacting regime via a Feshbach resonance, in which coupling between the lowest energy bands was dynamically generated [12]. Theoretically, Diener and Ho showed that a band insulator may evolve into a state with more bands occupied near the Feshbach resonance [13]. Very recently, Ho studied the phase transition from band insulator to Mott insulator for a fermionic system in optical lattices at a filling of two fermions per site under the two-band approximation [14]. In that work, the Hund-like orbital coupling term is shown to play a special role in the strongly interacting regime and favors spin alignment between different orbits.

It is thus physically nontrivial to go beyond the single-band approximation. Motivated by the recent progress in research into the atomic gas in an optical lattice near a Feshbach resonance, in this paper we study the equal mixing of a two-component boson in an optical lattice with a filling of two bosons per site, focusing on the Mott-insulating regime and the spin-related phase transition due to the Feshbach resonance. As in the fermionic case, on each site there are many orbits and higher orbits may be occupied when the system is near the Feshbach resonance. Without loss of generality and for the purpose of simplicity, we take into account only two bands in the following text, which can be fulfilled by enforcing an on-site interacting energy smaller than the energy level spacing between the third and the first orbital. We will show that in the strongly interacting regime the induced interband coupling prefers the two atoms in different orbits on a site to form an on-site singlet, which is quite different from the Hund-like orbital coupling in the fermionic systems [14]. For simplicity, we consider only a one-dimensional (1D) system which can be achieved by tuning the laser amplitudes $V_{0x} \ll V_{0y}, V_{0z}$ to produce a set of uncoupled 1D tubes [15,16]. In each tube, the system is effectively described by a 1D optical lattice because the transverse motion is completely frozen.

We start with the microscopic Hamiltonian of the two-component bosonic system in a 1D optical lattice

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$$H = \sum_{\sigma} \int_0^L dx \frac{\hbar^2}{2m} [\partial_x \psi_\sigma^\dagger(x) \partial_x \psi_\sigma(x)] + \sum_{\sigma} \int_0^L dx (V_{0x} \sin^2 kx - \mu_\sigma) \psi_\sigma^\dagger(x) \psi_\sigma(x) + \sum_{\sigma,\sigma'} \frac{c}{4} \int_0^L dx \psi_\sigma^\dagger(x) \psi_{\sigma'}^\dagger(x) \psi_{\sigma'}(x) \psi_\sigma(x), \quad (1)$$

where the spin indices $\sigma = \uparrow, \downarrow$ indicate the two species of atoms or, equivalently, atoms with two internal states, and μ_σ is the chemical potential. For the equally mixed bosons, we have $\mu_\uparrow = \mu_\downarrow = \mu$ corresponding to $N_\uparrow = N_\downarrow$, where N_σ is the total atom number of each species. The optical lattice potential has the form of $V_{0x} \sin^2 kx$ with wave vectors $k = 2\pi/\lambda$ and λ is the wavelength of the laser light. The parameter $c > 0$ describes the repulsive interaction of the atoms and the strengths of intraspecies and of interspecies interactions are taken to be the same. Since we are interested in the regime where the interaction energy is tuned so that at most two Bloch bands are populated, it is sufficient to expand the operator $\psi_\sigma(x)$ in the lowest two Wannier functions

$$\psi_\sigma(x) = \sum_{i,\alpha=1,2} \omega_{i\alpha}(x) c_{i\sigma\alpha}, \quad (2)$$

where the operator $c_{i\sigma\alpha}$ annihilates an atom with spin σ in the band α at lattice site i. In a deep lattice the Wannier functions $\omega_{i\alpha}(x)$ can be approximated by the local harmonic oscillator orbits in the ground state and the first excited state

$$\omega_{i1}(x) = \frac{1}{(\pi a_0^2)^{1/4}} \exp \frac{-(x - x_i)^2}{2a_0^2}, \quad (3)$$

$$\omega_{i2}(x) = \frac{(-1)^i}{(\pi a_0^2)^{1/4}} \frac{\sqrt{2}(x - x_i)}{a_0} \exp \frac{-(x - x_i)^2}{2a_0^2}, \quad (4)$$

where $a_0 = \sqrt{\hbar/m\omega_T}$ is the ground-state size of the local harmonic oscillator. Here $\omega_T = \sqrt{4V_{0x}E_R}/\hbar$ and $E_R = \hbar^2 k^2/2m$ is the recoil energy.

The second quantized Hamiltonian thus consists of three parts

$$H = H_t + H_{intra} + H_{inter}. \quad (5)$$

The hopping term H_t describes tunneling of atoms from one site to another, which is typically assumed to occur between the nearest neighboring sites

$$H_t = -\sum_{i,\sigma,\alpha,\beta} t_{\alpha\beta} c_{i+1\sigma\alpha}^\dagger c_{i\sigma\beta} + \text{H.c.}, \quad (6)$$

and the hopping energy is

$$t_{\alpha\beta} = -\frac{\hbar^2}{2m} \int_0^L dx \, \partial_x \omega_{i+1\alpha}(x) \partial_x \omega_{i\beta}(x). \quad (7)$$

H_{intra} is the contact-type interaction Hamiltonian in the same energy band,

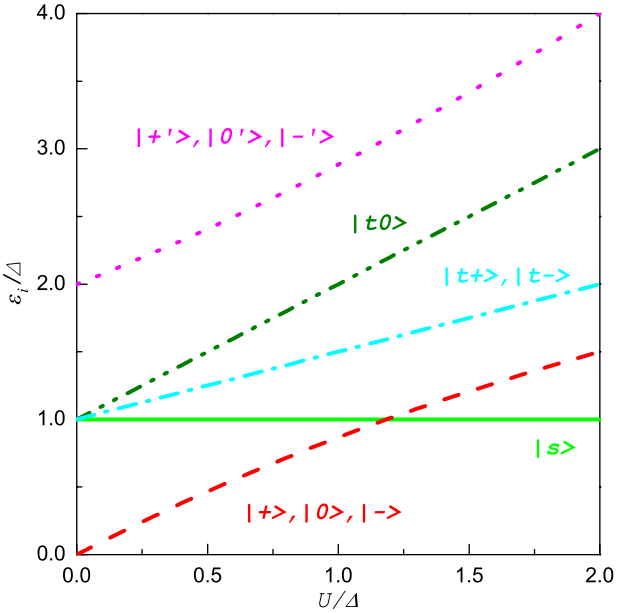

FIG. 1. (Color online) The on-site energies ε_i versus U/Δ where we have made a total energy shift of $-2\mu_1$.

$$H_{intra} = -\sum_{i,\sigma,\alpha} \mu_\alpha c_{i\sigma\alpha}^\dagger c_{i\sigma\alpha} + \sum_{i,\alpha} U_{\alpha\alpha} n_{i\uparrow\alpha} n_{i\downarrow\alpha} + \frac{1}{2} \sum_{i,\sigma,\alpha} U_{\alpha\alpha} n_{i\sigma\alpha} (n_{i\sigma\alpha} - 1), \quad (8)$$

where the chemical potentials for each band

$$\mu_\alpha = -\int_0^L dx \left(-\frac{\hbar^2}{2m} \partial_x^2 + V_{0x} \sin^2 kx - \mu \right) \omega_{i\alpha}^2(x) \quad (9)$$

are distinguished by a difference $\Delta = \mu_1 - \mu_2$. This difference is roughly the band gap between the two bands for deep lattice. On the other hand, the on-site interaction Hamiltonian between the two bands is denoted as H_{inter},

$$H_{inter} = \sum_{i,\alpha \neq \beta} U_{\alpha\beta} (n_{i\uparrow\alpha} n_{i\downarrow\beta} + S_{i\alpha}^+ S_{i\beta}^- + \Delta_{i\alpha}^\dagger \Delta_{i\beta}) + \frac{1}{2} \sum_{i,\sigma,\alpha \neq \beta} U_{\alpha\beta} (n_{i\sigma\alpha} n_{i\sigma\beta} + \Delta'_{i\sigma\alpha}{}^\dagger \Delta'_{i\sigma\beta}), \quad (10)$$

where $\Delta_{i\beta} = c_{i\downarrow\beta} c_{i\uparrow\beta}$, $\Delta'_{i\sigma\beta} = c_{i\sigma\beta} c_{i\sigma\beta}$, and $S_{i\alpha}^+ = c_{i\uparrow\alpha}^\dagger c_{i\downarrow\alpha}$ $[S_{i\alpha}^- = (S_{i\alpha}^+)^\dagger]$ is a pseudo-spin-operator. The repulsive interaction (positive scattering length) between two atoms sharing a lattice site in the same band or between the two bands gives rise to an interaction energy

$$U_{\alpha\alpha} = \frac{c}{2} \int_0^L dx \, \omega_{i\alpha}^4(x) \quad (11)$$

or

$$U_{12} = \frac{c}{2} \int_0^L dx \, \omega_{i1}^2(x) \omega_{i2}^2(x) = U_{21}, \quad (12)$$

which is just the additional energy that one needs to put two atoms on one site, in the same band or in different bands.

The term $S_{i\alpha}^{+}S_{i\beta}^{-}$ describes the orbital coupling between the upper and lower bands or orbits. A striking feature here is that we have got an interaction term with opposite sign compared to the fermionic case [14], for which the Hund-like orbital coupling term favors the spin of the two fermions at each site residing in different bands being aligned parallel. The orbital coupling thus determines the ground state in a different way for the bosonic case. The spins tend to align antiparallel in different bands when the interaction exceeds the energy gap far away as illustrated later in Fig. 2. The terms of $\Delta_{i\alpha}^{\dagger}\Delta_{i\beta}$ and $\Delta_{i\sigma\alpha}^{\prime}{}^{\dagger}\Delta_{i\sigma\beta}^{\prime}$ describe the interaction of atomic pairs in different bands.

Substituting the approximate Wannier functions Eqs. (3) and (4) into Eqs. (7), (11), and (12) we easily obtain the parameters $U_{11}=U, U_{22}=0.75U, U_{12}=0.5U$ where $U=c/4\sqrt{2\pi}a_0$. Unlike the long-range Coulomb interactions for electrons in solids, here the orbital coupling term is of the same order of magnitude as the on-site repulsion term. Owing to the approximation of local harmonic oscillator orbits on Wannier functions, the integral of the hopping matrix element between different bands is nonzero and in fact they satisfy the relations $|t_{11}|<|t_{12}|<|t_{22}|$. In optical lattice, both the hopping term $t_{\alpha\beta}$ and the on-site interaction U depend on the amplitude V_0 of the laser field. In this work, we will focus on the Mott phase with a larger ratio of $U/t_{\alpha\beta}$ and study the ground-state phase transition due to the change of the on-site interaction. In principle, via the Feshbach resonance, one could tune the strength of interaction so that $U<\Delta$ or $\Delta<U<2\Delta$. In the former case two bosons occupy the lowest Bloch band while in the latter case one of the atoms in the lowest band would be forced into the higher excited band.

In the strong coupling limit with $t_{\alpha\beta}\ll U_{\alpha\beta},\Delta$, it is instructive to first consider the on-site local Hamiltonian with $t_{\alpha\beta}=0$ and then treat the hopping term (6) as perturbation. It is easy to diagonalize the local on-site Hamiltonian [both intra- and interband parts (8) and (10)] with two bosons per site. The local spectra are given by

$$\varepsilon_1=-2\mu_1+\Delta+\frac{7U}{8}-\sqrt{\left(\Delta-\frac{U}{8}\right)^2+\left(\frac{U}{2}\right)^2},$$

$$\varepsilon_2=-2\mu_1+\Delta,$$

$$\varepsilon_3=-2\mu_1+\Delta+\frac{U}{2},$$

$$\varepsilon_4=-2\mu_1+\Delta+U,$$

$$\varepsilon_5=-2\mu_1+\Delta+\frac{7U}{8}+\sqrt{\left(\Delta-\frac{U}{8}\right)^2+\left(\frac{U}{2}\right)^2}.$$

Among the ten eigenstates, those corresponding to eigenenergy ε_1 are threefold degenerate and are given by

$$|+\rangle=-e|\uparrow\uparrow,0\rangle+f|0,\uparrow\uparrow\rangle,$$

$$|0\rangle=-e|\uparrow\downarrow,0\rangle+f|0,\downarrow\uparrow\rangle.$$

$$|-\rangle=-e|\downarrow\downarrow,0\rangle+f|0,\downarrow\downarrow\rangle.$$

The state corresponding to ε_2 is a local singlet formed by the atoms in the upper and lower orbits,

$$|s\rangle=\frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle).$$

The states corresponding to ε_3 are

$$|t+\rangle=|\uparrow,\uparrow\rangle,$$

$$|t-\rangle=|\downarrow,\downarrow\rangle,$$

and state corresponding to ε_4 is

$$|t0\rangle=\frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle).$$

Finally the states corresponding to ε_5 are again threefold degenerate,

$$|+'\rangle=f|\uparrow\uparrow,0\rangle+e|0,\uparrow\uparrow\rangle,$$

$$|0'\rangle=f|\uparrow\downarrow,0\rangle+e|0,\downarrow\uparrow\rangle,$$

$$|-'\rangle=f|\downarrow\downarrow,0\rangle+e|0,\downarrow\downarrow\rangle.$$

Here we have used the notation for the representation of eigenstates that the notation to the left of the comma is for band 1 and that to the right of the comma is for band 2. For example, $|\uparrow\uparrow,0\rangle=(1/\sqrt{2})(c_{\uparrow 1}^{\dagger})^2|0\rangle$ represents two atoms with spin of $\uparrow$ in the lower orbit and $|\uparrow,\downarrow\rangle=c_{\uparrow 1}^{\dagger}c_{\downarrow 2}^{\dagger}0\rangle$ represents an atom with spin of $\uparrow$ in the lower orbit and an atom with spin of $\downarrow$ in the upper orbit. The coefficients

$$e=\frac{1}{\sqrt{2}}\sqrt{1+\frac{1}{\sqrt{1+\left(\frac{1}{2\Delta/U-1/4}\right)^2}}},$$

$$f=\frac{1}{\sqrt{2}}\sqrt{1-\frac{1}{\sqrt{1+\left(\frac{1}{2\Delta/U-1/4}\right)^2}}},$$

satisfy $e^2+f^2=1$ and e^2 and f^2 describe the probability that two atoms simultaneously stay in the lowest band and the upper band, respectively. We have $0<f^2\lesssim 0.0659$ for $0<U<\Delta$. When $U/\Delta\to 0$, $f^2\to 0$ and thus the system goes back to the single-band model. To give concrete examples, we note that $f^2=0.0006$ for $U/\Delta=0.1$ and $f^2=0.0169$ for $U/\Delta=0.5$. Hence in the weakly interacting regime the two atoms mainly stay in the lowest band.

In Fig. 1, we display the five eigenenergies as a function of U/Δ. To get the phase diagram for the ground state, it is sufficient to identify the lowest two levels while ε_3, ε_4, and ε_5 always correspond to the higher bands. The competition of the lowest two levels gives rise to a completely different ground-state structure of the system and the transition point $U_c/\Delta\simeq 1.19$ is approximately determined by the energy level crossing of ε_1 and ε_2. For $U>U_c$, the local ground state on each site is a singlet state $|s\rangle$ with the spins of the two bosons

aligned antiparallel. For $U<U_c$, the local ground state is one of the spin triplet $|+\rangle$, $|0\rangle$, and $|-\rangle$. It is worthwhile to indicate that, although the total spin satisfies $\langle S_z^{total}\rangle=0$ as a result of $N_\uparrow=N_\downarrow$, at each site the two species of bosons are not necessarily equally mixed. At first sight, this seems to imply that, in the limit of $t_{\alpha\beta}=0$ and $U<U_c$, the ground state of the whole system is highly degenerate and the spins of atoms at each site align arbitrarily because the local ground state on an isolated site can be any of the three states as long as the total spin of the system is zero. Actually this is not true when the hopping processes between the neighboring sites are considered.

Now we switch on the hopping term between the nearest-neighbor sites. For the system with a filling factor of 2, the state with two atoms at each site has lowest on-site energy. The process of an atom hopping to its neighboring site would change the on-site population; however, such a hopping process is greatly suppressed because placing three atoms at a site costs a lot of energy. Nevertheless, the virtual process of hopping to an intermediate state and then hopping back gives a second-order correction to the ground-state energy and lowers the ground-state energy. The virtual hopping process does not change the total on-site populations but can exchange two different atoms on neighboring sites. These virtual exchange processes can be described by an effective Hamiltonian acting on the ground states which is obtained in second-order perturbation theory as

$$H_{eff}=\sum_{i,m}\frac{\langle\mu_{i,i+1}|H_t|m\rangle\langle m|H_t|\upsilon_{i,i+1}\rangle}{E_0-E_m}|\mu_{i,i+1}\rangle\langle\upsilon_{i,i+1}| \quad (13)$$

where $\{|\mu_{i,i+1}\rangle,|\upsilon_{i,i+1}\rangle=|g\rangle_i\otimes|g\rangle_{i+1}\}$ are ground-states with $N_i=N_{i+1}=2$ and with ground-state energy E_0. As $U<U_c$, the threefold-degenerate ground states at an isolated site form a triplet, i.e., $|g\rangle_i=|+\rangle_i,|0\rangle_i$, or $|-\rangle_i$, and therefore $|\mu_{i,i+1}\rangle$ is ninefold degenerate with $E_0=2\varepsilon_1$. In the opposite regime of $U>U_c$, $|\mu_{i,i+1}\rangle=|s\rangle_i\otimes|s\rangle_{i+1}$ with $E_0=2\varepsilon_2$. The intermediate states are the products of states on the two neighboring sites with three and one bosons, respectively, and with excitation energies E_m.

The second-order perturbation calculation of the hopping terms enables us to identify one type of spin-related quantum phase transition induced by the Feshbach resonance. On the one side of the transition point, that is, in the weakly interacting regime ($U<U_c$), the effective Hamiltonian can be further simplified and represented as an effective isotropic Heisenberg model in terms of spin-1 operators. After straightforward but tedious algebra we get the effective Hamiltonian

$$H_{eff}=-\lambda\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j \quad (14)$$

where S^α is a spin-1 operator in α ($\alpha=x,y,z$) orientation and the spin exchange coefficient is

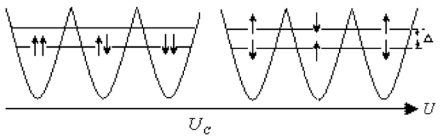

FIG. 2. Schematic picture for competing ground states in an optical lattice. A phase transition from spin exchange to bosonic singlet occurs at $U=U_c$.

$$\lambda=e^4\frac{2(t_{11})^2}{U}+2e^2f^2\left(\frac{(t_{12})^2}{\Delta+U}+\frac{(t_{12})^2}{3\Delta+\frac{1}{4}U}\right), \quad (15)$$

where the term f^4 is neglected due to its smallness. Equation (14) is nothing but the Hamiltonian of an isotropic $S=1$ ferromagnetic quantum Heisenberg spin system. In the limiting case $\Delta\gg U$, that is, when the upper band lies much higher than the lower band, we find

$$\lambda=2\frac{(t_{11})^2}{U}. \quad (16)$$

In this limit, the probability of two atoms occupying the lowest band e^2 approaches unity. We then recover the result in the single-band approximation [5,8]. The isotropic ferromagnetic model (14) has $(2S^{total}+1)$-fold degeneracy with $S^{total}=N/2$ ($N/2=N_\uparrow=N_\downarrow$). The ground state corresponds to the state with $S_z^{total}=0$, in which case no spatial broken symmetry occurs. In the bosonic language, this means that the system phase does not separate in the ground state for the SU(2)-symmetric model.

On the other side of the transition point, when $U>U_c$, the ground state at the isolated site is a singlet. In this case, the virtual hopping process does not induce redistribution of on-site spins and the global ground state is the product of on-site singlets. We straightforwardly obtain the correction to the ground-state energy per site of the optical lattice by calculating the virtual hopping process to second-order perturbation

$$\epsilon=\varepsilon_2+\delta\epsilon \quad (17)$$

with

$$\delta\epsilon=-\frac{3}{2}\left(\frac{(t_{11})^2}{2U}+\frac{(t_{22})^2}{\frac{7}{4}U}+\frac{(t_{12})^2}{\Delta+\frac{7}{4}U}+\frac{(t_{12})^2}{2U-\Delta}\right). \quad (18)$$

Obviously this correction is negative and the hopping process always lowers the ground state energy.

Figure 2 depicts the phase diagram of two- bosons in the two-band optical lattice model. For the interaction $U<U_c$, the atoms on a site form a triplet and the virtual hopping process produces ferromagnetic exchange between spins on neighboring sites, while in the strong coupling limit $U>U_c$ the atoms in different bands prefer to align their spins antiparallel and form an on-site singlet. A phase transition from spin exchange to bosonic singlet occurs therefore at $U=U_c$. We recall that in the fermionic case the phase diagram exhibits drastically different structure. Fermions with a filling factor 2 in a two-band optical lattice are shown to exhibit

opposite behavior and there exists a phase transition from the band insulator to a Mott insulator with interesting dynamics of a spin-1 Heisenberg antiferromagnet [14].

We notice here a big difference between 1D fermions and bosons. According to Haldane's conjecture, the ground state of SU(2)-symmetric antiferromagnetic spin-1 Hamiltonian is gapped. Hence, small deviations of the Hamiltonian parameters reducing the SU(2) symmetry to U(1) will not lead to qualitatively different results. On the other hand, the ground state for the ferromagnetic Hamiltonian is ordered and it is crucially important to consider a generic non-SU(2)-symmetric model in order to understand whether the ground state is an easy-axis or easy-plane ferromagnet.

To do this, we let the tunneling matrix elements $t_{\alpha\beta}^{\sigma}$ ($\sigma=\uparrow,\downarrow$) depend not only on band indices α,β but also on the component index σ. Furthermore we distinguish the intraspecies interaction $U=U_{\uparrow\uparrow}=U_{\downarrow\downarrow}$ and interspecies interaction $U'=U_{\uparrow\downarrow}$ to break the SU(2) symmetry. When the system is in the strongly interacting regime, deviation of the SU(2) symmetry does not lead to qualitative change of the ground state properties because the ground state is composed of on-site singlets. However, in the weakly interacting regime, when the SU(2) symmetry is broken, the effective Hamiltonian can be of the easy-axis type or of the easy-plane type with different kinds of ground states. We note that, for the general case with $U\neq U'$, the effective Hamiltonian cannot be represented in the form of a simple spin exchange model. However, if $|U'-U|\ll U,U'$, we can attribute the difference of the on-site interacting energies to the zeroth-order Hamiltonian [5] and get an effective Hamiltonian of the *XXZ* model

$$H=-\sum_{\langle i,j\rangle}[\lambda'\mathbf{S}_i\cdot\mathbf{S}_j+\delta\lambda_z' S_{iz}S_{jz}]+B\sum_i S_{iz}+D\sum_i (S_{iz})^2, \tag{19}$$

where

$$\lambda'=2e^4\frac{t_{11}^{\downarrow}t_{11}^{\uparrow}}{U}+2e^2f^2t_{12}^{\uparrow}t_{12}^{\downarrow}\left(\frac{1}{3\Delta+\frac{1}{4}U}+\frac{1}{\Delta+U}\right),$$

$$\delta\lambda_z'=e^4\frac{(t_{11}^{\uparrow}-t_{11}^{\downarrow})^2}{U}$$

$$+e^2f^2(t_{12}^{\uparrow}-t_{12}^{\downarrow})^2\left(\frac{1}{\Delta+U}+\frac{1}{3\Delta+\frac{1}{4}U}\right),$$

$$B=-e^4\left(3\frac{(t_{11}^{\uparrow})^2-(t_{11}^{\downarrow})^2}{U}+\frac{(t_{12}^{\uparrow})^2-(t_{12}^{\downarrow})^2}{\Delta}\right)$$

$$-e^2f^2\left(\frac{(t_{11}^{\uparrow})^2-(t_{11}^{\downarrow})^2}{2\Delta-\frac{1}{4}U}+\frac{(t_{22}^{\uparrow})^2-(t_{22}^{\downarrow})^2}{2\Delta}\right)$$

$$-3e^2f^2[(t_{12}^{\uparrow})^2-(t_{12}^{\downarrow})^2]\left(\frac{1}{3\Delta+\frac{1}{4}U}+\frac{1}{\Delta+U}\right)$$

and

$$D=\frac{7}{8}(U-U')-\sqrt{\left(\Delta-\frac{U}{8}\right)^2+\left(\frac{U}{2}\right)^2}$$

$$+\sqrt{\left(\Delta-\frac{U'}{8}\right)^2+\left(\frac{U'}{2}\right)^2}.$$

In the limiting case $\Delta\gg U$, it is easy to show that $\lambda'=2t_{11}^{\downarrow}t_{11}^{\uparrow}/U$, $\delta\lambda_z'=[t_{11}^{\uparrow}-t_{11}^{\downarrow}]^2/U$, $B=-3[(t_{11\uparrow})^2-(t_{11\downarrow})^2]/U$, and $D\approx U-U'$ and we recover the result for the single-band approximation [5,8]. It is obvious that we have always a positive small anisotropy parameter $\delta\lambda_z'$ for $t_{\alpha\beta}^{\uparrow}\neq t_{\alpha\beta}^{\downarrow}$, which implies that the effective *XXZ* model describes an easy-axis ferromagnet. Under the condition of $\delta\lambda_z'\gg D$, the ground state of the spin system is in a phase with spin domains. In the bosonic language, it corresponds to the situation with phase separation of the two components. This implies that differentiating the tunneling terms for different components would induce phase segregation. When $t_{\alpha\beta}^{\uparrow}=t_{\alpha\beta}^{\downarrow}$, we have $\delta\lambda_z'=0$ and $B=0$ which reduces the model to (14) except for an additional term D [which vanishes naturally for the SU(2)-symmetric model because $U=U'$]. For a large positive D, however, an easy-plane ground state can be realized. In terms of the nomenclature in Ref. [5], the easy-plane ferromagnet means a counterflow superfluid. Straightforwardly, a positive D reduces the S_z component of the spin on each site. At large enough $D>0$, all spins will be essentially confined to the state with $\langle S_{iz}\rangle=0$, which implies that a large enough intracomponent interaction ($U\gg U'$) leads to two atoms belonging to distinct species occupying each site. On the other hand, for small enough $D<0$ ($U\ll U'$), the ground state would stay in the state with $\langle S_{iz}\rangle=\pm 1$ and the term of D enhances the phase separation of different components.

Before ending the discussion, we would like to note the extension of the present work to the case with higher dimensions. Unlike the single-band model which can be directly extended to the high-dimensional case, the effective Hamiltonians (14) and (19) are no longer applicable to the high-dimensional optical lattice models when the higher orbits are populated. For higher dimensions, the first excited state in a local site is degenerate and has spatial anisotropy. Correspondingly, the hopping matrix element acquires spatial anisotropy and new physical phenomena may arise due to the orbital degeneracy [17–19].

In summary, we have studied the quantum phase transition induced by effective orbital coupling in optical lattices for an equally mixed two-component boson system at a filling factor of 2 per site. In the regime with weak on-site interaction, the two atoms stay in the lowest band and can be described by an effective spin-1 ferromagnetic exchange model. In the regime with strong on-site interaction, the two atoms prefer to occupy different orbits on a site and form an on-site singlet due to the effective orbital coupling. We also

considered the generic non-SU(2)-symmetry model. In the weakly interacting regime, the ground state may be described by an easy-axis ferromagnet corresponding to the case of phase separation or an easy-plane ferromagnet corresponding to the state of a counterflow superfluid.

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