Ground-state Competition of Two-Component Bosons in Optical Lattice near a Feshbach Resonance

Liping Guo,1,2 Yunbo Zhang,1,3 and Shu Chen2

1Department of Physics and Institute of Theoretical Physics, Shanxi University, Taiyuan 030006, P. R. China
2Institute of Physics, Chinese Academy of Sciences, Beijing 100080, P. R. China
3Laboratory of Optics and Spectroscopy, Department of Physics, University of Turku, 20014 Turku, Finland

We investigate the ground state properties of an equal mixture of two species of bosons in its Mott-insulator phase at a filling factor two per site. We identify one type of spin triplet-singlet transition through the competition of 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 tunnelling 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 \((U > U_c)\), 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 counter-flow superfluidity, respectively.

PACS numbers: 05.30.Jp, 03.75.Mn, 73.43.Nq

The study of quantum phase transition in optical lattices has made great progress both theoretically and experimentally \cite{1,2} and becomes one of focusing 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 \cite{1} and Greiner et. al. experimentally confirmed that the phase transition from superfluid phase to Mott-insulator could be realized by suppressing tunnelling between neighboring sites \cite{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 \cite{1,2,3}. When the spinless bosons are in the Mott phase, the on-site fluctuation of particle numbers is suppressed \cite{4}. Many studies have shown that multi-component bosonic or fermionic gases in optical lattices exhibit much richer phase diagrams \cite{1,2,3,4,5,6,7,8,9,10,11}. An intriguing feature of the multi-component 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 analogue in traditional condensed matter physics \cite{11}.

So far, a number of schemes have been proposed to derive an effective Hamiltonian to describe the spin-related dynamics for the multi-component system in the Mott-insulator phase \cite{7,8}. Most of the schemes ignore the existence of the upper bands and take 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 the 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 \cite{12}. Theoretically, Diener and T.-L. Ho analyzed that a band insulator may evolve into the state with more bands occupied near the Feshbach resonance \cite{13}. Very recently, A. F. 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 \cite{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 on the research of the atomic gas in optical lattice near a Feshbach resonance, in this paper we study the equal-mixing two-component bosons in 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 the 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 inter-band 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 \cite{14}. For simplicity, we consider only a one-dimensional
(1D) system which can be achieved by tuning the laser
amplitudes \( V_{0x}, V_{0y}, V_{0z} \) 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

\[
H = \sum_{\sigma} \int_0^L dx \frac{\hbar^2}{2m} \left( \partial_x \psi^\dagger_{\sigma} (x) \partial_x \psi_{\sigma} (x) \right) \\
+ \sum_{\sigma} \int_0^L dx \left( V_{0z} \sin^2 kx - \mu_{\sigma} \right) \psi^\dagger_{\sigma} (x) \psi_{\sigma} (x) \\
+ \sum_{\sigma,\sigma'} c \int_0^L dx \psi_{\sigma}(x) \psi_{\sigma'}(x) \psi_{\sigma'}(x) \psi_{\sigma}(x),
\]

(1)

where the “spin” indices \( \sigma = \uparrow, \downarrow \) indicate the two species
of atoms or, equivalently, atoms with two internal states
and \( \mu_{\sigma} \) is the chemical potential. For the equal-mixing
bosons, we have \( \mu_\uparrow = \mu_\downarrow = \mu \) corresponding to\( N_\uparrow = N_\downarrow \),
where \( N_\sigma \) is the total atom number of each specie. The
optical lattice potential has the form of \( V_{0z} \sin^2 kx \) with
wave vectors \( k = 2\pi/\lambda \) and \( \lambda \) the wavelength of the
laser light. The parameter \( c > 0 \) describes the repulsive
interaction of the atoms and the interaction strengths
of intra-species and of inter-species 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

\[
\psi_{\sigma} (x) = \sum_{i,\sigma=1,2} \omega_{i\sigma} (x) c_{i\sigma},
\]

(2)

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

\[
\omega_{i1} (x) = \frac{1}{\left( \pi a_0^2 \right)^{1/4}} \exp \left( -\frac{(x-x_i)^2}{2a_0^2} \right),
\]

\[
\omega_{i2} (x) = \frac{(-1)^i \sqrt{2} (x-x_i)}{\left( \pi a_0^2 \right)^{1/4}} \frac{(x-x_i)}{a_0} \exp \left( -\frac{(x-x_i)^2}{2a_0^2} \right),
\]

(3)

(4)

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

The second quantized Hamiltonian thus consists of three parts

\[
H = H_t + H_{\text{intra}} + H_{\text{inter}}.
\]

(5)

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

\[
H_t = - \sum_{i,\sigma,\alpha,\beta} t_{\alpha\beta} c_{i+1\sigma}^\dagger c_{i\alpha \beta} + H.c.,
\]

(6)

and the hopping energy is

\[
t_{\alpha\beta} = - \frac{\hbar^2}{2m} \int_0^L dx \partial_x \omega_{i+1\sigma} (x) \partial_x \omega_{i\beta} (x).
\]

(7)

\( H_{\text{intra}} \) is the contact-type interaction Hamiltonian in the same energy band

\[
H_{\text{intra}} = - \sum_{i,\sigma,\alpha} \mu_{\alpha} c_{i\sigma}^\dagger c_{i\alpha} + \sum_{i,\sigma} U_{\alpha\alpha} n_{i\sigma} n_{i\sigma} + \frac{1}{2} \sum_{i,\sigma,\alpha} U_{\alpha\alpha} n_{i\sigma} (n_{i\sigma} - 1),
\]

(8)

where the chemical potentials for each band

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

(9)

are distinguished by a difference \( \Delta = \mu_\uparrow - \mu_\downarrow \). This difference is roughly the band gap between the two bands for
dependent lattice. On the other hand, the on-site interaction
Hamiltonian between the two bands is denoted as

\[
H_{\text{inter}} = \sum_{i,\sigma,\alpha \neq \beta} U_{\alpha\beta} (n_{i\alpha} n_{i\beta} + S_{i\alpha}^+ S_{i\beta}^+ + \Delta_{i\alpha}^+ \Delta_{i\beta}) + \frac{1}{2} \sum_{i,\sigma,\alpha \neq \beta} U_{\alpha\alpha} (n_{i\sigma} n_{i\sigma} + \Delta_{i\sigma}^+ \Delta_{i\sigma})
\]

(10)

where \( \Delta_{i\beta} = c_{i\beta} c_{\beta i}, \Delta_{i\sigma}^+ = c_{i\sigma} c_{\sigma i}^\dagger \) and \( S_{i\alpha}^\dagger = c_{i\alpha}^\dagger c_{\alpha i} \). The 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

\[
U_{\alpha\alpha} = c \int_0^L dx \omega_{i\alpha}^2 (x) \omega_{i\alpha}^2 (x) = U_{21},
\]

(11)

or

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

(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 of \( S_{i\alpha}^+ S_{i\beta}^- \) describes the orbital coupling between the upper and lower bands/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 aligning paralleled. The orbital coupling
does thus determines the ground state in a different way for
the bosonic case. The spins tend to align anti-parallel
in different bands when the interaction exceeds the energy
gap far away as illustrated later in Figure 2. The terms of \( \Delta_{i\alpha}^+ \Delta_{i\beta} \) and \( \Delta_{i\sigma}^+ \Delta_{i\sigma}^\dagger \) describe the interaction
of atomic pair in different bands.
Substituting the approximate Wannier functions Eqs. (3) and (4) into (7), (11) and (12) we easily obtain the parameters $U_{11} = U, U_{22} = 0.75U, U_{12} = 0.5U$ where $U = e/4\sqrt{2}\pi a_0$. 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 $U/t$ 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 as perturbation. It is easy to diagonalize the local on-site Hamiltonian (both intra- and inter-band parts (8) and (10)) with two bosons per site. The local spectrum are given by:

$$\epsilon_1 = -2\mu_1 + \Delta + \frac{7U}{8} - \sqrt{\left( \Delta - \frac{U}{2} \right)^2 + \left( \frac{U}{2} \right)^2},$$

$$\epsilon_2 = -2\mu_1 + \Delta,$$

$$\epsilon_3 = -2\mu_1 + \Delta + \frac{U}{2},$$

$$\epsilon_4 = -2\mu_1 + \Delta + U,$$

$$\epsilon_5 = -2\mu_1 + \Delta + \frac{7U}{8} + \sqrt{\left( \Delta - \frac{U}{2} \right)^2 + \left( \frac{U}{2} \right)^2}.$$

Among the ten eigenstates, those corresponding to eigenenergy $\epsilon_1$ are three-fold degenerate and are given by

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

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

The state corresponding to $\epsilon_2$ is a local singlet forming 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 $\epsilon_3$ are

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

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

Finally the states corresponding to $\epsilon_4$ are again three-fold degenerate

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

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

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

Here we have used the notation for the representation of eigenstates that the left of comma in the right bar is for band 1 and the right of comma is for band 2. For example, $|\uparrow\downarrow, 0\rangle = \frac{1}{\sqrt{2}} (c_{\uparrow\downarrow1}^{\dagger} c_{\uparrow\downarrow2}^{\dagger} |0\rangle)$ represents two atoms with spin of $\uparrow$ in the lower orbit and $|\uparrow, \downarrow\rangle = c_{\uparrow\downarrow1}^{\dagger} c_{\uparrow\downarrow2}^{\dagger} |0\rangle$ represents an atom with spin of $\uparrow$ in the lower orbit and an atom with spin of $\downarrow$ in the upper orbit. The coefficients $e$ and $f$ fulfill $e^2 + f^2 = 1$ and $e^2$ and $f^2$ describe the probability two atoms simultaneously stay at the lowest band and the upper band respectively. We have $0 < f^2 \lesssim 0.0659$.
for $0 < U < \Delta$. When $U/\Delta \rightarrow 0$, \(f^2 \rightarrow 0\) and thus the system goes back to the single band model. To give concrete examples, we note \(f^2 = 0.0006\) 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 Figure 1, we display the five eigenenergies as a function of $U/\Delta$. To get the phase diagram for the ground state, it is sufficient to identify the lowest two levels while \(\varepsilon_3\), \(\varepsilon_4\) and \(\varepsilon_5\) always correspond to the higher bands. The competition of the lowest two levels gives rise to 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 \(\varepsilon_1\) and \(\varepsilon_2\). 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 antiparalleled. 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 fulfills \(\langle S_i^{(\text{total})}\rangle = 0\) as a result of \(N_\uparrow = N_\downarrow\), at each site the two species of bosons are not necessarily equal-mixing. At the 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 either 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 two, 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 extremely costs 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 exchanging processes can be described by an effective Hamiltonian acting on the ground states which is obtained in a second-order perturbation theory as

\[
H_{\text{eff}} = -\lambda \sum_{\langle i,j \rangle} S_i \cdot S_j
\]

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

\[
\lambda = e^2 \frac{2 (t_{11})^2}{U} + 2e^2 f^2 \left( \frac{(t_{12})^2}{\Delta + U} + \frac{(t_{12})^2}{3\Delta + 4U} \right).
\]

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

\[
H_{\text{eff}} = -\lambda \sum_{\langle i,j \rangle} S_i \cdot S_j
\]

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

\[
\lambda = e^2 \frac{2 (t_{11})^2}{U} + 2e^2 f^2 \left( \frac{(t_{12})^2}{\Delta + U} + \frac{(t_{12})^2}{3\Delta + 4U} \right).
\]

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

\[
H_{\text{eff}} = -\lambda \sum_{\langle i,j \rangle} S_i \cdot S_j
\]

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

\[
\lambda = e^2 \frac{2 (t_{11})^2}{U} + 2e^2 f^2 \left( \frac{(t_{12})^2}{\Delta + U} + \frac{(t_{12})^2}{3\Delta + 4U} \right).
\]

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

\[
H_{\text{eff}} = -\lambda \sum_{\langle i,j \rangle} S_i \cdot S_j
\]

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

\[
\lambda = e^2 \frac{2 (t_{11})^2}{U} + 2e^2 f^2 \left( \frac{(t_{12})^2}{\Delta + U} + \frac{(t_{12})^2}{3\Delta + 4U} \right).
\]
with
\[
\delta \epsilon = -\frac{3}{2} \left( \frac{(t_{11})^2}{2U} + \frac{(t_{22})^2}{4U} + \frac{(t_{12})^2}{\Delta + \frac{U}{4}} + \frac{(t_{12})^2}{2U - \Delta} \right).
\]
(18)

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

Figure 2 depicts the phase diagram of two-boson in 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 spin anti-paralleled 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 two in 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 anti-ferromagnet [14].

We notice here a big difference between 1D fermions and bosons. According to Haldane’s conjecture, the ground state for the ferromagnetic spin-1 Heisenberg anti-ferromagnet [14].

To do this, we let the tunnelling matrix elements \(t_{\sigma \alpha \beta}^{\sigma} (\sigma = \uparrow, \downarrow)\) depend not only on band indices \(\alpha, \beta\) but also on the component index \(\sigma\). Furthermore we distinguish the intra-species interaction \(U = U_{\uparrow \uparrow} = U_{\downarrow \downarrow}\) and inter-species 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 can not 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 and get an effective Hamiltonian of XXZ model

\[
H = -\sum_{(i,j)} [\lambda S_i \cdot S_j + \Delta \lambda_z S_i z S_j z] + B \sum_i S_{iz} + D \sum_i (S_{iz})^2,
\]
(19)

where
\[
\lambda' = 2e^2 f^2 t_{11}^+ t_{11}^- U + 2e^2 f^2 t_{12}^+ t_{12}^- \left( \frac{1}{3\Delta + \frac{1}{4}U} + \frac{1}{\Delta + U} \right),
\]
\[
\delta \lambda_z' = e^2 \left( \frac{t_{11}^+ - t_{11}^-}{U} + e^2 f^2 \left( \frac{t_{12}^+ - t_{12}^-}{\Delta} + \frac{1}{\Delta + U} \right) \right),
\]
\[
B = -e^4 \left[ \frac{3(t_{11}^+ - t_{11}^-)^2}{U} + \frac{(t_{12}^+ - t_{12}^-)^2}{\Delta} \right],
\]
\[
-3e^2 f^2 \left[ \frac{t_{11}^+ - t_{12}^-}{2\Delta - \frac{U}{4}} + \frac{t_{12}^+ - t_{12}^-}{2\Delta} \right]
\]
\[
D = \frac{7}{8} (U - U') - \sqrt{\left( \frac{\Delta - \frac{U}{8}}{2} \right)^2 + \left( \frac{U}{2} \right)^2}
\]

In the limiting case \(\Delta \gg U\), it is easy to show that \(\lambda' = 2t_{11}^+ t_{11}^- / U\), \(\delta \lambda'_z = [t_{11}^+ - t_{11}^-]^2 / U\), \(B = -3[(t_{11}^+)^2 - (t_{11}^-)^2] / U\) 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 \(t_{1\alpha \beta}^{\sigma} \neq t_{\alpha \beta \sigma}^{\sigma}\), which implies 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 \(t_{1\alpha \beta}^{\sigma} = t_{\alpha \beta \sigma}^{\sigma}\), we have \(\delta \lambda'_z = 0 \) and \(B = 0\) which reduces the model to except an additional term \(D\) (which vanishes naturally for \(SU(2)\)-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. [3], the easy-plane ferromagnet means the counter-flow 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 \((S_{iz}) = 0\), which implies that large enough intra-component 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 remark 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 \[17, 18, 19\].

In summary, we have studied the quantum phase transition induced by effective orbital coupling in optical lattices for an equal-mixing two-component boson system at a filling factor two 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 counter-flow superfluid.

S.C. is supported by NSF of China under Grant No. 10574150 and program of Chinese Academy of Science. Y.Z. is supported by Shanxi Province Youth Science Foundation under grant No. 20051001 and by Academy of Finland under grant number 206108.

[1] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. 81, 3108 (1998).
[2] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature 415, 39 (2002).
[3] D. van Oosten, P. van der Straten, and H. T. C. Stoof, Phys. Rev. A 63 053601 (2001).
[4] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B. 40 546 (1989).
[5] A. B. Kuklov and B. V. Svistunov, Phys. Rev. Lett. 90, 100401 (2003).
[6] A. Kuklov, N. Prokof’ev and B. Svistunov, Phys. Rev. Lett. 92, 050402 (2004).
[7] L.-M. Duan, E. Demler and M. D. Lukin, Phys. Rev. Lett. 91 090402 (2003).
[8] E. Altman, W. Hofstetter, E. Demler and M. D. Lukin, New J. Phys., 5, 113 (2003).
[9] M. A. Cazalilla, A. F. Ho, and T. Giamarchi, Phys. Rev. Lett. 95, 226402 (2005).
[10] C. Wu, J. P. Hu and S. C. Zhang, Phys. Rev. Lett. 91, 186402 (2005); S. Chen, C. Wu, S. C. Zhang and Y. Wang, Phys. Rev. B. 72, 214428 (2005).
[11] K. Winkler, G. Thalhammer, F. Lang, R. Grim, J. H. Denschlag, A. J. Daley, A. Kantian, H. P. Büchler, and P. Zoller, Nature 441, 853 (2006); L. Fallani and M. Inguscio, Nature 441, 820 (2006).
[12] M. Köhl, H. Moritz, T. Stöferle, K. Günter, and T. Esslinger, Phys. Rev. Lett. 94, 080403 (2005).
[13] R. B. Diener and T.-L. Ho, Phys. Rev. Lett. 96, 010402 (2006).
[14] A. F. Ho, Phys. Rev. A 73, 061601(R) (2006).
[15] H. Moritz, T. Stöferle, M. Köhl, and T. Esslinger, Phys. Rev. Lett. 91, 250402 (2003).
[16] H. Moritz, T. Stöferle, K. Günter, M. Köhl, and T. Esslinger, Phys. Rev. Lett. 94, 210401 (2005).
[17] A. Isacsson, and S. M. Girvin, Phys. Rev. A 72, 053604 (2005).
[18] A. B. Kuklov, Phys. Rev. Lett. 97, 110405 (2006).
[19] W. V. Liu and C. Wu, Phys. Rev. A 74, 013607 (2006).