Quantum Phase Transition of Spin-2 Cold Bosons in an Optical Lattice

Jing-Min Hou and Mo-Lin Ge

Theoretical Physics Division, Nankai Institute of Mathematics, Nankai University, Tianjin, 300071, China and Liuhui Center for Applied Mathematics, Tianjin, 300071, China

Abstract

The Bose-Hubbard Hamiltonian of spin-2 cold bosons with repulsive interaction in an optical lattice is proposed. After neglecting the hopping term, the site-independent Hamiltonian and its energy eigenvalues and eigenstates are obtained. We consider the hopping term as a perturbation to do the calculations in second order and draw the phase diagrams for different cases. The phase diagrams show that there is a phase transition from Mott insulator with integer number bosons to superfluid when the ratio $c_0/t$ ($c_0$ is the spin-independent on-site interaction and $t$ the hopping matrix element between adjacent lattice sites) is decreased to a critical value and that there is different phase boundary between superfluid and Mott insulator phase for different Zeeman level component in some ground states. We find that the position of phase boundary for different Zeeman level component is related to its average population in the Mott ground state.

PACS number(s):03.75.Kk, 03.75.Lm, 03.75.Mn, 32.80.Pj
I. INTRODUCTION

During recent years, the superfluid-Mott insulator transition becomes a significant topic of atomic physics, which has been extensively studied in the context of $^4$He absorbed in the porous media[1]. The detailed study of superfluid-Mott insulator transition becomes possible when quantum phase transition from a superfluid to a Mott insulating ground state was observed in a Bose-Einstein condensate stored in a three dimensional optical lattice potential by Greiner et al.[2]. The optical lattices used to confine cold atoms are induced by the ac Stark effect of interfering laser beams. The dynamics of the bosonic atoms in optical lattices realizes a Bose-Hubbard model[3], which predicts phase transition from a superfluid(SF) to Mott insulator(MI) at low temperature with increasing the ratio of the on site interaction $c_0$ to the hopping matrix element $t$.

Besides many experimental efforts made to realize superfluid-Mott insulator transition, a large number of theoretical literatures appeared[1, 3, 4, 5, 6, 7]. Ref. [4] made an appropriate mean-field approximation to the Hamiltonian of spinless or polarized bosons in an optical lattice to describe the zero-temperature phase transition from the superfluid to the Mott-insulating phase analytically and calculated the phase diagram. In this paper a first-order approximation to the dispersion of the density fluctuations shows that the system indeed goes from a gapped to a gapless phase.

Since trapping a Bose condensate by purely optical means is realized several years ago[8], which liberates the internal degrees of freedom of spinor Bosons that are frozen in a magnetic trap, much attention is attracted on the study of spinor Bose condensate, which has multiple components. Ho[9] and Ohmi and Machida[10] have researched a spin-1 BEC and obtained the general theoretical frameworks respectively. Ciobanu,Yip and Ho[11] have studied an $F = 2$ spinor bose condenate and drawn the phase diagrams. Koashi and Ueda have obtained the exact eigenstates of spin-1 and spin-2 vertical BEC and discussed their magnetic response[12, 13].

The next natural step after the detailed research of spinor bose condensates with free internal freedom is the study of the spinor multi-component BEC in a optical lattice—a new background. Demler and Zhou have studied spin-1 Bose atoms in an optical lattice and obtained several unique properties[6]. Ref. [7] studied the spin-1 bosons interacting antiferromagnetically in an optical lattice with the mean-field approximation method and obtained the phase diagram showing a transition from Mott insulator to superfluid, which is signed by the appearing of the superfluid order parameter i.e. the density fluctuations. But the spin-2 cold Bose atoms in an
optical lattice have not been researched as yet, which is the principal task of this paper.

In this paper, we study the transition from Mott insulator to superfluid of spin-2 Bose atoms with repulsive interaction in terms of mean-field approximation method. First, ignoring the hopping term of the Hamiltonian, we get the eigenstates and eigenvalues and find the ground states of the system for different cases. Then, we consider the hopping term as a perturbation to do calculations in second order and draw the phase diagrams.

II. THE MODEL

We consider bosons with hyperfine spin $F = 2$, such as $^{23}\text{Na}$, $^{87}\text{Rb}$ or $^{85}\text{Rb}$, in an optical lattice. Adding the external periodic potential term $V(\mathbf{r}) = V_0(\sin^2 kx + \sin^2 ky + \sin^2 kz)$, where $V_0$ is a tunable amplitude and $k$ the wave vector of the laser light, to the Hamiltonian of spin-2 bosons \[11\], we get the Hamiltonian of spin-2 bosons in an optical lattice in second quantized form as follows

$$H = \int d\mathbf{r} \left[ \frac{\hbar}{2m} \nabla \Psi_\alpha \cdot \nabla \Psi_\alpha + V(\mathbf{r}) \Psi_\alpha \Psi_\alpha - \mu \Psi_\alpha \Psi_\alpha + \frac{c_0}{2} \Psi_\alpha \Psi_\beta \Psi_\beta \Psi_\alpha + \frac{c_1}{2} \sum_i (\Psi_\alpha^\dagger (F_i)_{\alpha\beta} \Psi_\beta)^2 + c_2 \Psi_\alpha^\dagger \Psi_\alpha^\dagger \langle 2\alpha; 2\alpha'|00\rangle \langle 00|2\beta; 2\beta'| \Psi_\beta \Psi_\beta' \right]$$

where $m$ is the atomic mass, $\Psi_{+2}, \ldots, \Psi_{-2}$ are the five-component field operators corresponding to the sublevels $m_F = +2, \ldots, -2$ of the hyperfine state $F = 2$, $\mu$ is the chemical potential, $c_0$, $c_1$ and $c_2$ are related to s-wave scattering length $a_0, a_2$ and $a_4$ of the two colliding bosons with total angular momenta 0, 2 and 4 by $c_0 = 4\pi \hbar^2 (3a_4 + 4a_2)/7m$, $c_1 = 4\pi \hbar^2 (a_4 - a_2)/7m$ and $c_2 = 4\pi \hbar^2 (3a_4 - 10a_2 + 7a_0)/7m$, $< 2\alpha; 2\alpha'|00 >$ and $< 00|2\beta; 2\beta' >$ are Clebsch-Gordan coefficients. $F_\alpha (\alpha = x, y, z)$ are $5 \times 5$ spin matrices satisfying the commutation relation $[F_\alpha, F_\beta] = \varepsilon_{\alpha\beta\gamma} F_\gamma$. For a single atom in the periodic potential, the energy eigenstates are Bloch states. In the tight-binding limit, we can superpose the Bloch states to get a set of Wannier functions, which are localized on an individual lattice site. Expanding the field operators in the Wannier basis and keeping only the lowest vibrational states, $\Psi_\alpha = \sum_i b_{i\alpha} w(\mathbf{r} - \mathbf{r}_i)$, Eq. (1) reduces to the Bose-Hubbard Hamiltonian

$$H = -t \sum_{<i,j>} b_i^\dagger b_j - \mu \sum_i \hat{n}_i + \frac{c_0}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \frac{c_1}{2} \sum_i (\hat{F}_i^2 - 6\hat{n}_i) + \frac{2c_2}{3} \sum_i \hat{S}_i^+ \hat{S}_i^-$$

where $\hat{F}_i = b_i^\dagger F_{\alpha\beta} b_{i\beta}$, and $\hat{n}_i = \sum_\alpha b_{i\alpha}^\dagger b_{i\alpha}$. $t = -\int d\mathbf{r} w_i^\ast(\mathbf{r}) (-\hbar^2 \nabla^2 / 2m + V(\mathbf{r})) w_j(\mathbf{r})$ is the hopping matrix element between adjacent sites $i$ and $j$. $c_i$ is on-site inter-atom interaction.
defined by $c_i = \bar{c}_i \int d\mathbf{r} |w_i(\mathbf{r})|^4$, where the Hubbard approximation has been used to approximate the multi-center integral as a single-center one. $\mathbf{S}_{i+} = \mathbf{S}_{i-} = (b_{i0}^\dagger)^2/2 - b_{i1}^\dagger b_{i-1}^\dagger + b_{i2}^\dagger b_{i-2}^\dagger$, when applied to the vacuum, creates a spin-singlet “pairs”. The properties of the operators will be discussed in detail in the following section. The fourth and fifth terms in the equation are adding terms comparing with the Bose-Hubbard Hamiltonian of spinless or polarized bosons. By contrast with that of spin-1 bosons, the fifth term is an adding term and $6\hat{n}_i$ in the fourth term replaces $2\hat{n}_i$.

In the limit $c_0/t \rightarrow \infty$, the hopping term in the Hamiltonian can be neglected, so the Hamiltonian is reduced to a diagonal matrix with respect to sites. Omitting the site index, the singe-site Hamiltonian is

$$h_0 = -\mu \hat{n} + \frac{c_0}{2} \hat{n} (\hat{n} - 1) + \frac{c_1}{2} (\hat{F}^2 - 6\hat{n}) + \frac{2c_2}{5} \hat{S}_+ \hat{S}_-$$

whose eigenstates and eigenvalues will be discussed in following section.

To study the quantum transition, we use the mean-field approximation to the hopping term and consider it as a perturbation. Here we introduce the superfluid order parameter $\phi_\alpha = \langle b_\alpha \rangle = \sqrt{n_{sf}} \zeta_\alpha$, where $n_{sf}$ is the superfluid density and $\zeta_\alpha$ is a normalized spinor $\zeta_\alpha^* \zeta_\alpha = 1$. The hopping term is decoupled as $b_\alpha^\dagger b_j = (\phi_\alpha b_\alpha^\dagger + \phi_\alpha^* b_j) - \phi_\alpha^* \phi_\alpha$. So the total hopping term becomes the product of a site-independent term and the total number of the sites. We can consider only a single site because the Hamiltonian of every site is identical in the homogenous case. In the single site, the resulting mean-field version of the hopping Hamiltonian can be written as

$$h_1 = zt (\phi_\alpha b_\alpha^\dagger + \phi_\alpha^* b_\alpha - \phi_\alpha^* \phi_\alpha)$$

where $z$ is the number of the nearest-neighbor sites and the site-index is omitted. So the Hamiltonian of a single site is

$$h = h_0 + h_1$$

When the ratio $c_0/t$ is very large, we can consider $h_1$ as a perturbative term.

III. THE ENERGY EIGENVALUES AND THE GROUND STATES

Before perturbative calculations we should get the eigenvalues and eigenstates of Eq.(3), i.e., to sovle the equation

$$h_0 \psi = \varepsilon^{(0)} \psi$$
In Eq. (3), the operators \( \hat{S}_+ \) and \( \hat{S}_- \) satisfy the \( SU(1,1) \) commutation relations together with 
\[
\hat{S}_z \equiv (2\mathcal{N} + 5)/4,
\]
and the Casimir operator \( \hat{S}^2 \) commuting with \( \hat{S}_\pm \) and \( \hat{S}_z \) reads
\[
\hat{S}^2 \equiv -\hat{S}_+ \hat{S}_- + \hat{S}_z^2 - \hat{S}_z
\]
The eigenvalues of the mutual eigenstates for \( \hat{S}^2 \) and \( \hat{S}_z \) are \( \{S(S - 1), S_z\} \) with \( S = (2n_0 + 5)/4 \) (\( n_0 = 0, 1, 2, \ldots \)) and \( S_z = S + n_s \) (\( n_s = 0, 1, 2, \ldots \)), which guarantees that \( \hat{S}_+ \hat{S}_- - \hat{S}_z^2 \) is positive semidefinite. The new quantum numbers \( n_s \) and \( n_0 \) are introduced and the operator \( S_z \) raises \( n_s \) by one while the relation \( n = 2n_s + n_0 \) holds, where \( n \) is the total number of bosons in a single site.

The operators \( \hat{S}_\pm \) commute with the spin operator \( \hat{F} \) and the magnetic quantum number operator \( \hat{F}_z \), so the energy eigenstates can be classified according to quantum numbers \( n_0 \) and \( n_s \), total spin \( F \), and magnetic quantum number \( F_z \). Hence, the eigenstates \( \psi \) are denoted as \( |n_0, n_s, F, F_z; \lambda> \) where \( \lambda \) labels orthonormal degenerate states. The energy eigenvalue is given by
\[
\varepsilon^{(0)} = -\mu n + \frac{c_0}{2} n(n - 1) + \frac{c_1}{2} [F(F + 1) - 6n] + \frac{2c_2}{5} n_s(n - n_s + \frac{3}{2})
\]
where the relation \( n = 2n_s + n_0 \) is used. So Mott states can be expressed as \( \prod_i |n_0, n_s, F, F_z; \lambda> \), where \( i \) is lattice site index. For homogenous case, the zeroth order total energy is \( E^{(0)} = \sum_i \varepsilon^{(0)} = N_1 \varepsilon^{(0)} \) where \( N_1 \) is the number of lattice sites.

From Ref. [13] we know that the energy eigenstates \( |n_0, n_s, F, F_z; \lambda> \) can be represented as
\[
(\hat{F}_-)^{\Delta F} (\hat{A}_0^{(2)\dagger})^{n_{20}} (\hat{A}_2^{(2)\dagger})^{n_{22}} (\hat{A}_0^{(3)\dagger})^{n_{30}} (\hat{A}_3^{(3)\dagger})^{n_{33}} |\text{vac}> \]
where
\[
\hat{A}_0^{(2)\dagger} = \frac{1}{\sqrt{10}} [(b_0^\dagger)^2 - 2b_0^\dagger b_{-1}^\dagger + 2b_{-2}^\dagger b_{-1}^\dagger] \quad \hat{A}_2^{(2)\dagger} = \frac{1}{\sqrt{14}} [2\sqrt{2}b_0^\dagger b_{-1}^\dagger - \sqrt{3}(b_1^\dagger)^2] \quad \hat{A}_0^{(3)\dagger} = \frac{1}{\sqrt{210}} [3\sqrt{2}(b_0^\dagger)^3 - 3\sqrt{2}b_0^\dagger b_{-1}^\dagger + 3\sqrt{3}(b_1^\dagger)^2 b_{-2}^\dagger + 3\sqrt{3}b_2^\dagger (b_{-1})^2 - 6\sqrt{2}b_0^\dagger b_{-1}^\dagger b_{-2}^\dagger] \quad \hat{A}_3^{(3)\dagger} = \frac{1}{20} [(b_1^\dagger)^3 - \sqrt{6}b_0^\dagger b_{-1}^\dagger + 2(b_{-2}^\dagger)^2 b_{-1}^\dagger]
\]
\( P_{(n_s=0)} \) is the projection onto the subspace with \( n_s = 0; n_{12}, n_{20}, n_{22}, n_{30} = 0, 1, 2, ..., \infty, n_{33} = 0, 1, \) and \( \Delta F = 0, 1, ..., 2F \) that are related to \( \{n_0, n_s, F, F_z\} \) as

\[
\begin{align*}
n_0 &= n_{12} + 2n_{22} + 3n_{30} + 3n_{33} \quad (15) \\
n_s &= n_{20} \quad (16) \\
F &= 2n_{12} + 2n_{22} + 3n_{33} \quad (17) \\
F_z &= F - \Delta F \quad (18)
\end{align*}
\]

To find the ground states of Eq.(3), we minimize its energy eigenvalue, i.e., Eq.(9). We note that there isn’t magnetic quantum number \( F_z \) in Eq.(9), which means the eigenstates with different magnetic quantum number but the same other quantum numbers are degenerate. For simplicity, in this paper we only investigate the states with the highest magnetic quantum number, i.e. the states with \( F_z = F \). when \( n = 1 \), it is obvious that the ground state is \( |1, 0, 2, 2; \lambda> \), which means only one single atom with the highest magnetic quantum number for the state. For \( n \geq 2 \), it is more complicated, which will be discussed in detail as follow:

1. \( c_1 > 0, \ c_2 > 0 \). In this case, if \( n_s = 0 \) and \( F = 0 \), the energy eigenvalue has its minimum. But that is not always the case because there are some forbidden values [12, 13], i.e., \( F = 1, 2, 5, 2n_0 - 1 \) are not allowed when \( n_0 = 3k(k \in Z) \), and \( F = 0, 1, 3, 2n_0 - 1 \) are forbidden when \( n_0 = 3k \pm 1(k \in Z) \), according to which, it is classified into three cases.

   (a) For \( n = 3k(k \in Z) \), \( |n, 0, 0, 0; \lambda> \) with \( n_s = 0 \) and \( F = 0 \) simultaneously, which is not within forbidden values, is the ground state

   (b) For \( n = 3k - 1(k \in Z) \), the state with \( n_s = 0 \) and \( F = 0 \) simultaneously is not allowed. If \( n_s = 0 \), the lowest allowed value of total spin \( F \) is 2. \( F = 0 \) is not forbidden when \( n_0 = 3k(k \in Z) \). \( n_s = 1 \), due to the relation \( n = 2n_s + n_0 \), is the lowest value satisfying the condition. So the state with \( n_s = 1 \) and \( F = 0 \) is a possible ground state. There is competition between the third term and the fourth term in Eq.(10), i.e., competition between contributions of total spin and singlet “pairs” to eigenenergy. Comparing both eigenenergies for the two cases \( F = 0, n_s = 1 \) and \( F = 2, n_s = 0 \), we get the ground state, (i)\( |n - 2, 1, 0, 0; \lambda> \) for \( c_1 > c_2(2n + 1)/15 \) and (ii) \( |n, 0, 2, 2; \lambda> \) for \( c_1 < c_2(2n + 1)/15 \).

   (c) For \( n = 3k + 1(k \in Z) \), it is similar to last case that there is competition between contributions of total spin and the singlet “pair” to eigenenergy in this case. But
there is a difference between the two cases in that if $F = 0$, $n_s$ is at least 2. Therefore, the ground state is (i) $|n-4, 0, 2, 2; \lambda >$ for $c_1 > 2c_2(2n-1)/15$; (ii) $|n, 0, 2, 2; \lambda >$ for $c_1 < 2c_2(2n-1)/15$, which is obtained by comparing the eigenenergy of these states.

2. $c_1 > 0, \ c_2 < 0$. In this case, the eigenenergy is the lowest when $F$ is at the lowest value and $n_s$ at the highest value. There is a state with $F = 0$ and $n_s = n/2$ when $n$ is even, but there is not when $n$ is odd. So, when $n$ is different, there are two cases as follow:

(a) When $n$ is even, the ground state is $|n, n/2, 0, 0; \lambda >$

(b) When $n$ is odd, $n_s$ has the highest value $(n-1)/2$. But $F$ is not zero when $n_s = (n-1)/2$. Alternatively, there is another case that $F = 0$ and $n_s = (n-3)/2$. In the two cases, the state that has lower eigenenergy is the ground state. Hence, the ground state is (i) $|1, (n-1)/2, 2, 2; \lambda >$ for $c_1 < 7|c_2|/15$; (ii) $|3, (n-3)/2, 0, 0; \lambda >$ for $c_1 > 7|c_2|/15$.

3. For $c_1 < 0, \ c_2 > 0$, the eigenstate with $F = 2n$ and $n_s = 0$, which has the lowest eigenenergy, is the ground state. So the ground state is $|n, 0, 2n, 2n; \lambda >$.

4. For $c_1 < 0, \ c_2 < 0$, to get the ground state, we minimize Eq. (19). If we skip over the fact for the moment that the singlet “pair” number $n_s$ is an integer, then the condition to minimize the energy function is given by

$$n_s = \frac{10c_1(4n + 1) - c_2(2n + 3)}{80c_1 - 4c_2}$$  \hspace{1cm} (19)$$

because of the fact that the singlet “pair” number must be an integer, we write $n_s$ in terms of the closet integer number $n_s^0$ and the decimal part, i.e. $n_s = n_s^0 + \alpha$, where the number $\alpha$ satisfy $-1/2 < \alpha < 1/2$, which can be rewritten as,

$$n_s^0 - \frac{1}{2} < \frac{10c_1(4n + 1) - c_2(2n + 3)}{80c_1 - 4c_2} < n_s^0 + \frac{1}{2}$$  \hspace{1cm} (20)$$

(a) Because the singlet “pair” number isn’t negative, for $n_s^0 < 0$, $n_s$ must be zero. Hence, in this case, the ground state is $|n, 0, 2n, 2n; \lambda >$.

(b) $0 < n_s^0 < \frac{n}{2}$. In this case, the eigenenergy is lower when the singlet “pair” number is $n_s^0$ than any other integer. So the ground state is $|n-2n_s^0, n_s, 2n-4n_s^0, 2n-4n_s^0; \lambda >$. 

7
(c) For $n_s^0 > \frac{n}{2}$, the singlet “pair” number takes the highest value as it can. With different total bosons number, there are two cases as follow: (i) when $n$ is even, the ground state is $|0, n/2, 0, 0; \lambda>$; (ii) when $n$ is odd, the ground state is $|1, n/2, 2, 2; \lambda>$.

IV. THE SUPERFLUID-MOTT INSULATOR TRANSITION

In this section, we consider the hopping term and calculate the first and second order corrections to the ground energy. Although the eigenstates, among whose quantum numbers only magnetic quantum number is different, are degenerate, we can do perturbative calculations regarding the degenerate states as nondegenerate ones for the off-diagonal hopping matrix elements between states with the same Boson number $n$ are zero, i.e., $< n_0, n_s, F, F_z; \lambda| h_1| n_0, n_s, F, F'_z; \lambda > = 0$, when $F_z \neq F'_z$. Therefore, the first and second order corrections to ground energy are expressed as follow

$$\varepsilon_g^{(1)} = < g| h_1| g > = z t \sum_\alpha \phi_\alpha^* \phi_\alpha \quad \alpha = -2, ..., 2$$

$$\varepsilon_g^{(2)} = \sum_{n \neq g} \frac{|< g| h_1| n >|^2}{\varepsilon_g^{(0)} - \varepsilon_n^{(0)}} = \sum_{n \neq g} \frac{z^2 t^2}{\varepsilon_g^{(0)} - \varepsilon_n^{(0)}} |< g| h_1| n >|^2 \phi_\alpha^* \phi_\alpha \quad \alpha = -2, ..., 2$$

The ground energy modified by adding the first and second order corrections becomes

$$\varepsilon_g = \varepsilon_g^{(0)} + \varepsilon_g^{(1)} + \varepsilon_g^{(2)} = \varepsilon_g^{(0)} + z t \sum_\alpha A_\alpha(n, \bar{\mu}, \bar{c}_0, \bar{c}_1, \bar{c}_2)\phi_\alpha^* \phi_\alpha \quad \alpha = -2, ..., 2$$

where $A_\alpha(n, \bar{\mu}, \bar{c}_0, \bar{c}_1, \bar{c}_2)$ is related to the first and second order corrections of the spin component with magnetic quantum number $\alpha$ to zero-order ground energy. It depends on $n$, $\bar{\mu}$, $\bar{c}_0, \bar{c}_1, \bar{c}_2$, where $\bar{\mu} = \mu/zt$, $\bar{c}_0 = c_0/zt$, $\bar{c}_1 = c_1/zt$, $\bar{c}_2 = c_2/zt$. Minimizing the ground energy function modified in second order, we find that $\phi_\alpha = 0$ when $A_\alpha(n, \bar{\mu}, \bar{c}_0, \bar{c}_1, \bar{c}_2) > 0$ and that $\phi_\alpha \neq 0$ when $A_\alpha(n, \bar{\mu}, \bar{c}_0, \bar{c}_1, \bar{c}_2) < 0$. This means that $A_\alpha(n, \bar{\mu}, \bar{c}_0, \bar{c}_1, \bar{c}_2) = 0$ signifies the boundary between the superfluid and the Mott insulator phases of the spin component with magnetic quantum number $\alpha$.

Equipping the perturbative calculations we can draw phase diagrams. The phase diagrams show that there is a phase transition from Mott insulator with integer number bosons to superfluid when the ratio $c_0/t$ is decreased to a critical value. In the zeroth order, i.e., neglecting the hopping term, the ground state is Mott state in which the occupation number per site is pinned at integer $n = 1, 2, ...$, corresponding to a commensurate filling of the lattice. Different Mott ground states maybe contain different spin components. For example, there is only spin...
component with Zeeman level \( m = 2 \) when occupation number per site \( n = 1 \); spin components with \( m = 0, \pm 1, \pm 2 \) for Mott state \( \prod_i (\hat{A}_0^{(2)} | 0 >)_i \) and spin components with \( m = 0, 1, 2 \) for \( \prod_i (\hat{A}_2^{(2)} | 0 >)_i \). It is easy to realize that only one superfluid component appears when lowering the ratio \( c_0/t \) for the initial Mott ground state containing only one spin component such as the case \( n = 1 \) in Fig.4 and \( n = 1, 2, 3 \) in Fig.5. For the Mott ground states containing multiple spin components, when lowering the ratio \( c_0/t \), multiple superfluid components appear. The phase boundaries between superfluid and Mott insulator phase for different spin components are identical for some Mott ground states such as \( n = 2 \) in Fig.1,3,4,6. and \( n = 3 \) in Fig.1,2,4, and different for some Mott ground states such as \( n = 2 \) in Fig.2 and \( n = 3 \) in Fig.3,6.

We find that the position of phase boundary is related to average occupation number of spin component in the initial Mott ground state, i.e., the larger the average occupation number of spin component per site is, the easier the transition from Mott insulator to superfluid phase. For example, in Fig.1 the average occupation numbers of spin component with Zeeman level \( m = 2 \) are 1, 2/5 and 3/5 per site for \( n = 1, 2, 3 \) Mott ground states respectively, and the minimum critical value of \( c_0 \) are 5.42zt, 2.76zt and 3.54zt for \( n = 1, 2, 3 \) Mott states. We can arrive at the same result by analyzing other figures.

V. CONCLUSION

In this paper, we have investigated the quantum phase transition from Mott insulator to superfluid phase of spin-2 cold bosons at zero temperature. First, we diagonalized the Bose-Hubbard Hamiltonian without hopping term and got the eigenvalue and ground states. Then taking the hopping term as a perturbation we calculated the first and second order corrections and drawn the phase diagrams, which show that there is a phase transition from Mott insulator with integer number bosons at each site to superfluid phase when the ratio \( c_0/t \) is decreased to a critical value. Different Mott ground states maybe contain different spin components. For some Mott ground states, the different spin components appear at different moment in superfluid phase when lowering the ratio \( c_0/t \). The position of phase boundary is related to average occupation number of spin component in the initial Mott ground state.
Acknowledgments

This work is in part supported by NSF of China No.A0124015.

[1] M.P.A.Fisher, P.B.Weichman, G.Grinstein, and D.S.Fisher, Phys.Rev. B 40, 546(1989)
[2] M.Greiner et al., Nature 415,39(2002)
[3] D.Jaksch, C.Bruder, J.I.Cirac, C.W.Gardiner, and P.Zoller, Phys.Rev.Lett. 81, 3108(1998)
[4] D.van Oosten, P.van der Straten, and H.T.C.Stoof, Phys. Rev. A 63, 053601(2001)
[5] G.H.Chen and Y.S.Wu Phys. Rev. A 67, 013606(2003)
[6] E.Demler and F.Zhou, Phys. Rev. Lett. 88, 163001(2002)
[7] S.Tsuchiya, S.Kurihara, and T.Kimura, cond-mat/0209676
[8] D.M.Stamper-Kurn et al., Phys.Rev.Lett. 80, 2027(1998)
[9] T.L.Ho, Phys. Rev. Lett. 81, 742(1998)
[10] T.Ohmi and K.Machida, J. Phys. Soc. Jpn. 67, 1822(1998)
[11] C.V.Ciobanu, S.K.Yip and T.L.Ho, Phys. Rev. A 61, 033607(2000)
[12] M.Koashi and M.Ueda, Phys. Rev. Lett. 84, 1066(2000)
[13] M.Ueda and M.Koashi, Phys. Rev. A 65, 063602(2002)
FIG. 1: Phase diagram of Bose-Hubbard Hamiltonian obtained from second-order perturbation theory with solid lines for $c_1 = 0.1\, t$ and $c_2 = 0.1\, t$. Here $c_0/zt$ and $\mu/zt$ are dimensionless. The dashed lines indicate the zeroth order phase diagram. In the diagram, SF and MI denote superfluid phase and Mott insulator phase respectively.
FIG. 2: Phase diagram of Bose-Hubbard Hamiltonian obtained from second-order perturbation theory with solid lines for $c_1 = 0.02 z t$ and $c_2 = 0.1 z t$. Here $c_0 / z t$ and $\mu / z t$ are dimensionless. The dashed lines indicate the zeroth order phase diagram. In the diagram, SF and MI denote superfluid phase and Mott insulator phase respectively. For $n = 2$, the interior line is the phase boundary of spin component with Zeeman level $m = 1$, and the external double lines, which are too close to be distinguished in the diagram, are that of spin components with $m = 0, 2$ respectively. The inset shows an expansion of the part of the phase boundaries for $n = 2$ in the dotted frame labelled by A.
FIG. 3: Phase diagram of Bose-Hubbard Hamiltonian obtained from second-order perturbation theory with solid lines for $c_1 = 0.02\, zt$ and $c_2 = -0.1\, zt$. Here $c_0/zt$ and $\mu/zt$ are dimensionless. The dashed lines indicate the zeroth order phase diagram. In the diagram, SF and MI denote superfluid phase and Mott insulator phase respectively. For $n = 3$ case, the interior line is the phase boundary of spin component with Zeeman level $m = 2$; the middle line the phase boundary of spin component with Zeeman level $m = -2$, and the external triple lines, which are too close to be distinguished in the diagram, the phase boundaries of spin components with Zeeman level $m = 0, \pm 1$. The inset shows an expansion of the part of the phase boundaries for $n = 3$ in the dotted frame labelled by B.
FIG. 4: Phase diagram of Bose-Hubbard Hamiltonian obtained from second-order perturbation theory with solid lines for $c_1 = 0.1zt$ and $c_2 = -0.1zt$. Here $c_0/zt$ and $\mu/zt$ are dimensionless. The dashed lines indicate the zeroth order phase diagram. In the diagram, SF and MI denote superfluid phase and Mott insulator phase respectively.
FIG. 5: Phase diagram of Bose-Hubbard Hamiltonian obtained from second-order perturbation theory with solid lines for $c_1 = -0.1zt$ and $c_2 = 0.1zt$. Here $c_0/zt$ and $\mu/zt$ are dimensionless. The dashed lines indicate the zeroth order phase diagram. In the diagram, SF and MI denote superfluid phase and Mott insulator phase respectively.
FIG. 6: Phase diagram of Bose-Hubbard Hamiltonian obtained from second-order perturbation theory with solid lines for $c_1 = -0.02 zt$ and $c_2 = -0.1 zt$. Here $c_0/zt$ and $\mu/zt$ are dimensionless. The dashed lines indicate the zeroth order phase diagram. In the diagram, SF and MI denote superfluid phase and Mott insulator phase respectively. For $n = 3$ case, the interior line is the phase boundary of spin component with Zeeman level $m = 2$; the middle line the phase boundary of spin component with Zeeman level $m = -2$, and the external triple lines, which are too close to be distinguished in the diagram, the phase boundaries of spin components with Zeeman level $m = 0, \pm 1$. The inset shows an expansion of the part of the phase boundaries for $n = 3$ in the dotted frame labelled by C.