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A t–J_1–J_2 model of spin-1 bosons in optical lattices

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Abstract
A t–J_1–J_2 model is constructed to describe the spin-1 bosons in optical lattices in the strong correlation limit. In the parameter region of $J_1 < J_2$, with the slave-boson-mean-field approach, it is found that two kinds of condensed phases may exist: a condensate with spin singlet pairs and a condensate with ferro-quadruple long range order coexisting with singlet pairs. A first-order quantum phase transition occurs at the point $J_1 = 0$. The finite-temperature phase transition in a cubic optical lattice was also discussed.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The optical lattice creates a convenient environment for studying the strongly correlated systems of cold atoms. It also provides an ideal platform to simulate conventional condensed matter systems because a variety of physical parameters, such as the interactions among the atoms, the dimensions of the system, the bandwidth and even the internal degrees of freedom of the particles, can be exactly controlled. More importantly, with a pure optical trap, it becomes possible to study the cold atoms with higher hyperfine spins.

For the spinor bosons, because the freedom of spin is released in optical traps, the ground state of the systems splits into different phases with different spin configurations. Compared to the other high spin boson systems the property of spin-1 bosons in an optical lattice is much simpler and fundamental. In fact, the research of spin-1 bosons in an optical lattice has been underway for many years. Experimentally, BEC of the cold atoms with hyperfine spin $F = 1$ have been achieved [1, 2] and the transition from superfluid to Mott insulator has also been observed in the spin-1 cold atom system in an optical lattice [3]. Much work on theory has been done on this aspect [4–6]. Different from that of spinless bosons, the ground state of high spin (in this paper, spin-1) boson systems have richer structure. For the spin-1 Bose condensate in an optical lattice, a polar state and ferromagnetic state were proposed by Ho [4]. Spin singlet states and spin nematic states were investigated by Zhou [5].

Even so, most of the previous studies still focused on the Mott phase or the weakly correlated condensation phase and spin-1 boson systems with fractional filling factor in an optical lattice were seldom touched. In this paper, we concentrate ourselves on the BEC state of spin-1 bosons in both square and cubic optical lattices in the strong correlation limit. The ground state of this system will remain in BEC naturally. As the t–J model for spin-$\frac{1}{2}$ fermions can be constructed from the Hubbard model in the large-U limit [7], we will construct a similar model (t–J_1–J_2 model) to describe the spin-1 boson system with fractional filling factor in the same large-U limit (here, U_0 and U_2). The structure of the present paper is organized as follows: in the subsequent section, we construct the model Hamiltonian from the spinor boson Hubbard model [4, 6]. A slave-boson-mean-field approach is applied to this model in section 3. As in the spin-$\frac{1}{2}$ t–J model [8], spin singlet boson pairs may exist in the condensate. In addition, a quantum phase transition is found and the finite-temperature phase transition in the cubic lattice is derived. A discussion and concluding remarks are given in the last section.

2. The model

We start our problem from the spin-1 Bose–Hubbard model in an optical lattice [4, 6]:

$$H = -t \sum_{\langle i,j\rangle,\alpha} (a^\dagger_{i,\alpha} a_{j,\alpha} + \text{h.c.}) + \frac{U_0}{2} \sum_i n_i(n_i - 1) + \frac{U_2}{2} \sum_i (\mathbf{S}_i^2 - 2n_i) - \mu \sum_i n_i, \quad (1)$$

where $a^\dagger_{i,\alpha}$ is the creation operator of atoms with spin component α on site i; n_i and $\mathbf{S}_i$ are the atom number and spin operators on site i, respectively; μ denotes the

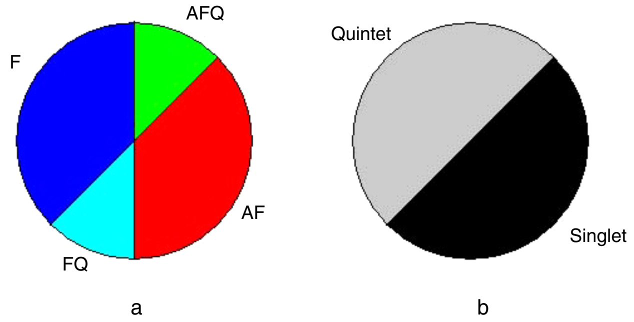

Figure 1. (a) The phase diagram of the SBBM model in square and cubic lattices with $J_1 = -\cos\varphi$, $J_2 = -\sin\varphi$. F represents ferromagnetic phase, AF is the antiferromagnetic phase, FQ means the ferro-quadruple long range order phase and AFQ is the antiferro-quadruple long range order phase. (b) The parameter regions favor quintet and singlet pairs. When $J_2 > J_1$ $(-\frac{3\pi}{4} < \varphi < \frac{\pi}{4})$ singlet pairs are favorable. When $J_2 < J_1$ $(\frac{\pi}{4} < \varphi < \frac{5\pi}{4})$ quintet pairs are favorable. Our concentration is on the singlet pair region (black).

chemical potential and t is the hopping integral of atoms between two nearest-neighbor sites; U_0 and U_2 are the Hubbard repulsion constants of atoms in the spin-0 and spin-2 channels, respectively; $\langle i, j\rangle$ denotes the nearest neighbor. The scattering channel of total spin $S = 1$ is prohibited because of the symmetry requirement of the wavefunctions. In the case of $t \ll U_0, U_2$, we can treat the t terms in the Hamiltonian (1) as a perturbation. Up to the second-order perturbation expansion, we get the effective interaction of atoms as [9]

$$H_{\text{int}} = J_0 \sum_{\langle i,j\rangle} n_i n_j - J_1 \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j - J_2 \sum_{\langle i,j\rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \quad (2)$$

with $J_1 = \frac{2t^2}{U_2}$, $J_2 = \frac{2t^2}{3U_2} + \frac{4t^2}{3U_0}$, and $J_0 = J_2 - J_1$. The above expression is quite similar to that of the t–J model. However, in the spin-$\frac{1}{2}$ systems non-trivial scattering only occurs in the spin singlet channel and a term of $\mathbf{S}_i \cdot \mathbf{S}_j$ is enough to describe the spin correlation, while in our case an additional term of $(\mathbf{S}_i \cdot \mathbf{S}_j)^2$ must be included to describe the extra non-trivial scattering in the spin-2 channel. The whole model Hamiltonian is

$$\begin{aligned} H = & -t \sum_{\langle i,j\rangle,\alpha} P a^\dagger_{i,\alpha} a_{j,\alpha} P + J_0 \sum_{\langle i,j\rangle} n_i n_j \\ & - J_1 \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j - J_2 \sum_{\langle i,j\rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \end{aligned} \quad (3)$$

where $P \cdots P$ means the single occupation condition $n_i \leqslant 1$. Exactly at $n_i = 1$, the model becomes the so-called spin-1 bilinear–biquadratic model (SBBM). The SBBM has been studied for many years and it presents a rich phase diagram with the variation of J_1/J_2. By setting $J_1 = -\cos\varphi$, $J_2 = -\sin\varphi$, the phase diagram can be given with the variation of the angle φ. In 1D, we do not get agreement on the phase diagram in the region of $-\frac{3\pi}{4} < \varphi < -\frac{\pi}{2}$. Whether in this region there exists a phase transition from a nematic state to a dimer state is still controversial [9–11]. In 2D or 3D, the most acceptable phase diagram [10, 12, 13] is shown in figure 1(a).

Obviously, the quantum states of each single site in the new Hamiltonian are projected to be either empty or singly occupied states. It is convenient to adopt the following slave-boson representation: $a^\dagger_{i,\alpha} \to a^\dagger_{i,\alpha} f_i$, $a_{i,\alpha} \to f^\dagger_i a_{i,\alpha}$, where $a^\dagger_{i,\alpha}$ and $f^\dagger_i$ are the particle and hole creation operators on site i, respectively. Both $a^\dagger_{i,\alpha}, a_{i,\alpha}$ and $f^\dagger_j, f_j$ obey the boson commutation relations. In this representation, the constraint condition $\sum_\alpha a^\dagger_i a_i \leqslant 1$ can be expressed as

$$\sum_\alpha a^\dagger_{i,\alpha} a_{i,\alpha} + f^\dagger_i f_i = 1.$$

The effective Hamiltonian (3) can be written as

$$\begin{aligned} H = & -t \sum_{\langle i,j\rangle,\alpha} (f^\dagger_j f_i a^\dagger_{i,\alpha} a_{j,\alpha} + \text{h.c.}) + J_0 \sum_{\langle i,j\rangle} n_i n_j \\ & - J_1 \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j - J_2 \sum_{\langle i,j\rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \\ & - \lambda \sum_i \left(1 - \sum_\alpha a^\dagger_{i,\alpha} a_{i,\alpha} - f^\dagger_i f_i\right) \end{aligned} \quad (4)$$

where λ is the Lagrangian multiplier. There should also be a chemical potential term here, but in the mean-field theory we used below these two terms have the same effect and we combine the chemical potential term into the Lagrangian term. In this model, two atoms on two nearest-neighbor sites may form a bound pair. The boson pair can be either a spin singlet or a spin quintet. We use (3) to calculate the energy of a two-site unit:

$$\begin{aligned} H|0,0\rangle &= J_0 + 2J_1 - 4J_2|0,0\rangle, \\ H|1,m_1\rangle &= 0, \\ H|2,m_2\rangle &= J_0 - 2J_1 - J_2|2,m_2\rangle, \end{aligned} \quad (5)$$

where in $|S, m_s\rangle$ S is the total spin of the two atoms and m_s is the magnetism of the total spin. For some atoms, if $U_0 < U_2 (J_1 < J_2)$ (like ^{23}Na), it is favorable for adjacent bosons to form singlet pairs. If $U_0 > U_2 (J_1 > J_2)$ (like ^{87}Rb), quintet pairs are more favorable. In this paper we concentrate on the singlet pairs. The region of singlet pairs with parameter φ is given in figure 1(b).

3. Slave-boson-mean-field approach

We introduce three boson operators [13, 14]:

$$\begin{aligned} b_{i1} &= \frac{1}{\sqrt{2}}(a_{i,-1} - a_{i,1}) \\ b_{i2} &= \frac{-\mathrm{i}}{\sqrt{2}}(a_{i,-1} + a_{i,1}) \\ b_{i3} &= a_{i,0}. \end{aligned} \quad (6)$$

The representation of the $SU(3)$ algebra can be expressed as

$$\begin{aligned} S_i^x &= -i(b_{i2}^\dagger b_{i3} - b_{i3}^\dagger b_{i2}), \\ S_i^y &= -i(b_{i3}^\dagger b_{i1} - b_{i1}^\dagger b_{i3}), \\ S_i^z &= -i(b_{i1}^\dagger b_{i2} - b_{i2}^\dagger b_{i1}), \\ Q_i^0 &= \tfrac{1}{3}(b_{i1}^\dagger b_{i1} + b_{i2}^\dagger b_{i2} - 2b_{i3}^\dagger b_{i3}), \\ Q_i^2 &= -i(b_{i1}^\dagger b_{i1} - b_{i2}^\dagger b_{i2}), \\ Q_i^{xy} &= -(b_{i1}^\dagger b_{i2} + b_{i2}^\dagger b_{i1}), \\ Q_i^{yz} &= -(b_{i2}^\dagger b_{i3} + b_{i3}^\dagger b_{i2}), \\ Q_i^{xz} &= -(b_{i1}^\dagger b_{i3} + b_{i3}^\dagger b_{i1}). \end{aligned} \tag{7}$$

The first three operators $\{S_i^x, S_i^y, S_i^z\}$ are the spin operators and the others $\{Q_i^0, Q_i^2, Q_i^{xy}, Q_i^{yz}, Q_i^{xz}\}$ are the quadrupole operators of the spin-1 bosons on site i. In the new representation, the Hamiltonian can be expressed as

$$\begin{aligned} H = &-t\sum_{\langle i,j\rangle,\alpha}(f_j^\dagger f_i b_{i,\alpha}^\dagger b_{j,\alpha} + \text{h.c.}) + J_0\sum_{\langle i,j\rangle} n_i n_j \\ &- \sum_{\langle i,j\rangle}\sum_{\alpha,\beta}[J_1 b_{i,\alpha}^\dagger b_{i,\beta} b_{j,\beta}^\dagger b_{j,\alpha} \\ &+ (J_2 - J_1) b_{i,\alpha}^\dagger b_{i,\beta} b_{j,\alpha}^\dagger b_{j,\beta}] \\ &- \lambda\sum_i\left(1 - \sum_\alpha b_{i,\alpha}^\dagger b_{i,\alpha} - f_i^\dagger f_i\right). \end{aligned} \tag{8}$$

For the Hamiltonian (3), there are two $SU(3)$-invariant points: $\varphi = -\frac{3\pi}{4}$ and $\frac{\pi}{4}$. At these two points, there is no quadruple order, i.e. $\langle Q\rangle = 0$. The analysis shows that in the parameter range of $-\frac{3\pi}{4} < \varphi < \frac{\pi}{4}$ the bosons prefer to form singlet pairs. In addition, ferro-quadruple order is also favored in this region. Those allow us to do the following mean-field approximations:

$$\begin{aligned} d_\alpha &= -\langle b_{i\alpha}^\dagger b_{j\beta}\rangle, \\ Q_1 &= -\langle b_{i1}^\dagger b_{i2} + b_{i2}^\dagger b_{i1}\rangle, \\ Q_2 &= -\langle b_{i2}^\dagger b_{i3} + b_{i3}^\dagger b_{i2}\rangle, \\ Q_3 &= -\langle b_{i1}^\dagger b_{i3} + b_{i3}^\dagger b_{i1}\rangle, \\ \langle f_i^\dagger\rangle &= \langle f_i\rangle = \sqrt{\delta}, \end{aligned}$$

where $\beta = 1, 2, 3$, δ is the hole density. Considering the $SU(2)$ symmetry of the Hamiltonian, we set $d_1 = d_2 = d_3$ and $Q_1 = Q_2 = Q_3$. With these approximations, the Hamiltonian can be diagonalized as

$$\begin{aligned} H = &\sum_k [E_{k1}(\alpha_1^\dagger\alpha_1 + \alpha_2^\dagger\alpha_2 + \alpha_3^\dagger\alpha_3 + \alpha_4^\dagger\alpha_4) \\ &+ E_{k2}(\alpha_5^\dagger\alpha_5 + \alpha_6^\dagger\alpha_6)] + \sum_k(2E_{k1} + E_{k2} - \tfrac{3}{2}a) \\ &+ \tfrac{3}{2}z(3J_2 - 4J_1)d^2N + \tfrac{3}{2}zJ_1Q^2N \\ &- \tfrac{1}{2}z(1-\delta)^2N - \lambda(1-\delta)N, \end{aligned} \tag{9}$$

where

$$E_{k1} = \tfrac{1}{2}\sqrt{(a-c)^2 - b^2},$$

$$E_{k1} = \tfrac{1}{2}\sqrt{(a+2c)^2 - b^2},$$

$$a = -tz\delta\gamma_k + J_0z(1-\delta) + \lambda,$$

$$b = (3J_2 - 4J_1)zd\gamma_k$$

$$c = zJ_1Q,$$

with $\gamma_k = \frac{2}{z}(\cos k_x + \cos k_y + \cos k_z)$ ($z = 6$) for the cubic lattice and $\gamma_k = \frac{1}{2}(\cos k_x + \cos k_y)$ ($z = 4$) for the square lattice. The free energy and the ground state energy are

$$\begin{aligned} G = &\sum_k 2K_BT\left\{2\ln\left[\cosh\left(\frac{E_{k1}}{2K_BT}\right)\right]\right. \\ &\left.+ \ln\left[\cosh\left(\frac{E_{k2}}{2K_BT}\right)\right]\right\} \\ &- \tfrac{3}{2}a + \tfrac{3}{2}zJ_1Q^2N + \tfrac{3}{2}z(3J_2 - 4J_1)d^2N \\ &- \tfrac{1}{2}z(1-\delta)^2N - \lambda(1-\delta)N, \\ E_g = &\sum_k(2E_{k1} + E_{k2} - \tfrac{3}{2}a) + \tfrac{3}{2}z(3J_2 - 4J_1)d^2N \\ &+ \tfrac{3}{2}zJ_1Q^2N - \tfrac{1}{2}z(1-\delta)^2N - \lambda(1-\delta)N. \end{aligned} \tag{10}$$

Minimizing the free energy leads to the following self-consistent equations:

$$\begin{aligned} \frac{5}{2} - \delta = &\frac{1}{N}\sum_k\left[\frac{a-c}{2E_{k1}}\coth\left(\frac{E_{k1}}{2K_BT}\right)\right. \\ &\left.+ \frac{a+2c}{4E_{k2}}\coth\left(\frac{E_{k2}}{2K_BT}\right)\right], \\ Q = &\frac{1}{3N}\sum_k\left[\frac{a-c}{2E_{k1}}\coth\left(\frac{E_{k1}}{2K_BT}\right)\right. \\ &\left.- \frac{a+2c}{2E_{k2}}\coth\left(\frac{E_{k2}}{2K_BT}\right)\right] \\ 1 = &\frac{1}{6N}(3J_2 - 4J_1)z\sum_k\gamma_k^2\left[\frac{1}{E_{k1}}\coth\left(\frac{E_{k1}}{2K_BT}\right)\right. \\ &\left.+ \frac{1}{2E_{k2}}\coth\left(\frac{E_{k2}}{2K_BT}\right)\right]. \end{aligned} \tag{11}$$

Away from the Mott phase, BEC always occurs in the ground state with a finite doping ratio. In the strong correlation limit ($t \ll U_0, U_2$), we find the BEC happens at $k = (0, 0)$ in 2D and $k = (0, 0, 0)$ in 3D. We set n_0 as the atom number density occupied on zero momentum. By separating the n_0 term from the summation, (n_0, Q, d) can be derived from the self-consistent equations when $T = 0$. The number of singlet pairs in the condensate can be estimated as

$$\sum_{k,\alpha} b_{k\alpha}^\dagger b_{-k\alpha}^\dagger b_{-k\alpha} b_{k\alpha} = \sum_\alpha\left[\sum_{k\neq 0} n_{k,\alpha}n_{-k,\alpha} + n_{0,\alpha}(n_{0,\alpha} - 1)\right]. \tag{12}$$

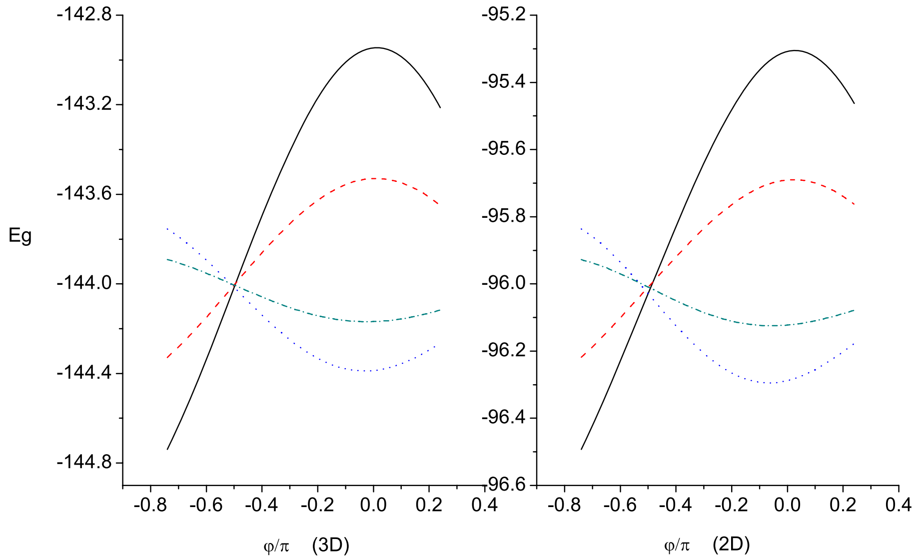

Figure 2. Ground state energy versus hole density δ. The solid (black) and dashed (red) lines represent the strong coupling pairing (SCP) phase with doping $\delta = 0.4, 0.6$. The dotted (blue) and dash-dotted (green) lines represent the spin singlet condensate (SSC) phase with $\delta = 0.4, 0.6$.

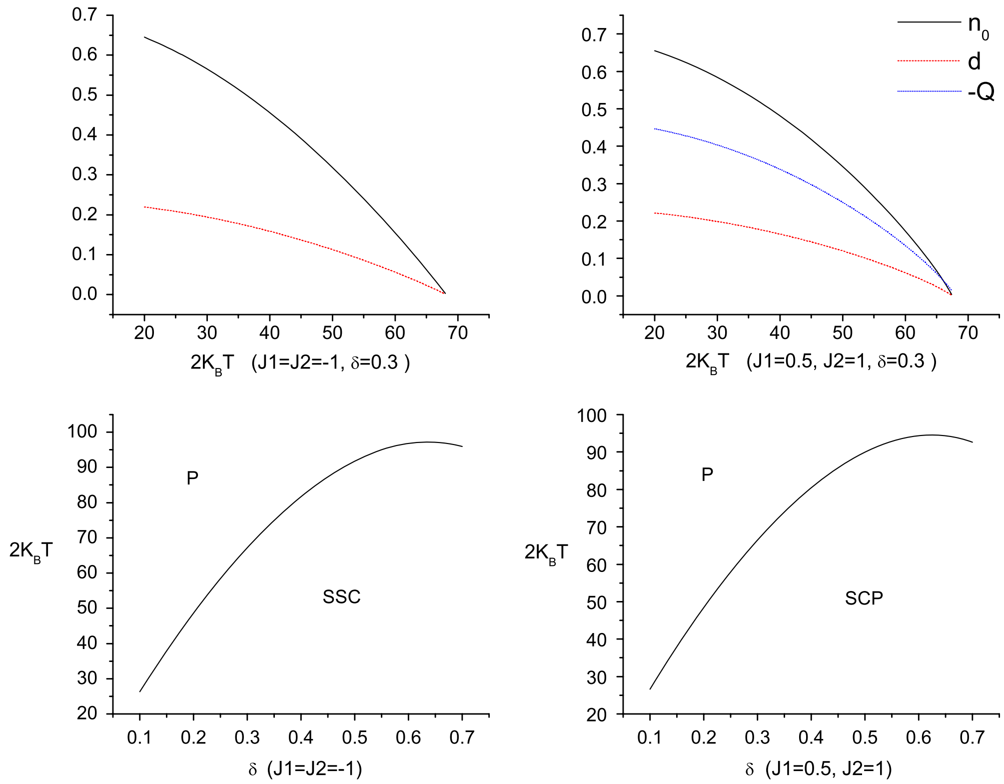

Figure 3. The order parameters with the change of temperature with fixed J_1, J_2, δ and the critical temperature with the change of δ for fixed J_1, J_2. In the left two figures, $J_1 = J_2 = -1$, $Q = 0$ and in the right two figures $J_1 = 0.5$, $J_2 = 1$, $Q \neq 0$. P represents the paramagnetic phase. SSC and SCP represent the spin singlet condensate and the strong coupling pairing phase.

Obviously, the singlet pair density is always finite in the condensate. In the ground state $T = 0$, the self-consistent equations have two solutions: $Q = 0$ and $Q \neq 0$. From the numerical result (figure 2), we find in 2D and 3D in the parameter range of $-\frac{3\pi}{4} < \varphi < -\frac{\pi}{2}$, $Q \neq 0$ corresponds to lower energy; while in the parameter range of $-\frac{\pi}{2} < \varphi < \frac{\pi}{4}$ $Q = 0$ gives lower energy. In the ground state

$$\langle b_k^\dagger b_k \rangle = \langle b_{i2}^\dagger b_{i2} \rangle = \langle b_{i3}^\dagger b_{i3} \rangle = \tfrac{1}{3},$$

indicating $\langle Q_i^2 \rangle = \langle Q_i^0 \rangle = 0$. This result shows that there is a quantum phase transition at $\varphi = -\frac{\pi}{2}$. For $-\frac{3\pi}{4} < \varphi < -\frac{\pi}{2}$

the ground state is a Bose–Einstein condensate with a ferro-quadruple long range order. It is just the so-called strong coupling pairing phase (SCP) [15] in which both $SO(3)$ and $U(1)$ symmetry are broken. For $-\frac{\pi}{2} < \varphi < \frac{\pi}{4}$ the ground state is a pure spin singlet condensate [15, 16] without quadruple order. In this phase only the $U(1)$ symmetry is broken but not $SO(3)$. Both two phases may correspond to the fragmented BEC in a Bose gas. By checking several filling ratios we find that the quantum critical point is unchanged.

In the cubic lattice, there is also a finite-temperature phase transition. We increase the temperature for fixed δ, t, J_1 and J_2, finding the order parameters of the singlet pairs and the usual BEC end at the same temperature (figure 3). The temperature of the phase transition with different doping ratio for fixed t, J_1 and J_2 is also shown in figure 3.

4. Discussion and concluding remarks

It is interesting to compare the present model and the usual fermion t–J model. In the usual t–J model, spin exchange between two adjacent particles is antiferromagnetic and only spin singlet Cooper pairs may exist. At least at the mean-field level, there is a competition between the antiferromagnetic phase and the superconducting phase in the ground state and the quantum phase transition occurs at a certain doping ratio. However, in the present model two adjacent spin-1 bosons may form either singlet or quintet pairs depending on J_1 and J_2. Besides, the condensate may have a ferro-quadruple order and the quantum phase transition occurs at a fixed parameter point independent of the filling ratio.

In summary, to study the spin-1 boson system in optical lattices in the strong correlation limit, we construct a t–J_1–J_2 model. In some parameter regions, it is found that the spin singlet pairs are favorable and coexist with the condensate. In addition, long range ferro-quadruple order may coexist with the condensate. A quantum phase transition in the condensate is also derived.

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References

[1] Stenger J *et al* 1999 *Nature* **396** 345
[2] Barrett M D, Sauer J A and Chapman M S 2001 *Phys. Rev. Lett.* **87** 010404
[3] Greiner M *et al* 2002 *Nature* **415** 39
[4] Ho T L 1998 *Phys. Rev. Lett.* **81** 742
[5] Zhou F and Snoek M 2003 *Ann. Phys.* **308** 692
[6] Tsuchiya S, Kurihara S and Kimura T 2004 *Phys. Rev.* A **70** 043628
[7] Hirsch J E 1985 *Phys. Rev. Lett.* **54** 1317
[8] Kotliar G and Liu J 1988 *Phys. Rev.* B **38** 5142
[9] Yip S K 2003 *Phys. Rev. Lett.* **90** 250402
[10] Fáth G and Sólyom J 1995 *Phys. Rev.* B **51** 3620
[11] Ivanov B A and Kolezhuk A K 2003 *Phys. Rev.* B **68** 052401
[12] Chubukov A V 1990 *J. Phys.: Condens. Matter* **2** 1593
[13] Li P, Zhang G M and Shen S Q 2007 *Phys. Rev.* B **75** 104420
[14] Zhang G M and Yu Lu 2005 *Preprint* cond-mat/0507158
[15] Demler E and Zhou F 2002 *Phys. Rev. Lett.* **88** 163001
[16] Zhou F and Snoek M 2003 *Preprint* cond-mat/0306697