First-order superfluid-Mott insulator transition of spinor bosons in an optical lattice

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Abstract

We study the superfluid-Mott insulator transition of antiferromagnetic spin-1 bosons in an optical lattice described by a Bose-Hubbard model. Our variational study with the Gutzwiller-type trial wave function determines that the superfluid-Mott insulator transition is a first-order one at a part of the phase boundary curve, contrary to the spinless case. This first-order transition may be observed through an experiment, such as a Stern-Gerlach type, under a magnetic field.

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Superfluid (SF) transition is one of the most striking phenomena of condensed matter physics. In particular, critical phenomena of superfluid transition, including the order of the transition, have been extensively studied for several decades. The quantum superfluid-Mott insulator (SF-MI) transition has been studied in granular superconductors [1], Josephson-junction arrays [2], and helium absorbed in the porous media [3]. Recently, the SF-MI transition of bosons in an optical lattice has been very clearly observed [4]. Jaksch *et al.* [5] have shown that bosons in an optical lattice can be described by a Hubbard model [6] (a Bose-Hubbard model). The Bose-Hubbard model for spinless bosons has been theoretically studied for the last two decades [6, 7, 8, 9, 10]. Monte Carlo studies [7] have confirmed that the transitions of the clean and dirty Bose-Hubbard models of spinless bosons are continuous as suggested by analytical studies [6].

It is also interesting to study the Bose-Hubbard model of spinor bosons [11]. Demler and Zhou [12] have discussed several unique properties of spin-1 bosons in an optical lattice. In a previous paper [13], we determined the SF-MI phase boundary of spin-1 bosons with an antiferromagnetic interaction using a perturbative mean-field approximation (PMFA) [9], which gives a phase boundary close to that obtained by Monte Carlo studies for the case of spinless bosons.

An excellent trial wave function for studying the Bose-Hubbard model is a Gutzwiller-type wave function (GW) [14], which has been frequently used for the Hubbard model for electrons [15]. For spinless bosons, the GW describes a second-order SF-MI transition and obtains a phase boundary curve, which is in an exact agreement with that obtained using the PMFA [9]. A GW for spinor bosons has been employed only recently for a non-uniform system [16].

In the present study, by employing the GW, we show the SF-MI transition can be a first-order one at a part of the phase boundary. The first-order SF-non-SF transition is rare and interesting. For example, as stated above, the SF-MI transition of the spinless bosons is second-order one [6]. Hence, the spin degree of freedom has an essential role in the first-order transition. The first-order transition can be observed by experiments, such as Stern-Gerlach type, under a magnetic field.

The Bose-Hubbard Hamiltonian [12, 17, 18] of spin-1 bosons is given by $H = H_0 + H_1$,

$$
\begin{aligned}
H_0 &= -t \sum_{\langle i,j \rangle} \sum_\alpha (a_{i\alpha}^\dagger a_{j\alpha} + a_{j\alpha}^\dagger a_{i\alpha}), \\
H_1 &= -\mu \sum_i \sum_\alpha a_{i\alpha}^\dagger a_{i\alpha} + \frac{1}{2} U_0 \sum_i \sum_{\alpha,\beta} a_{i\alpha}^\dagger a_{i\beta}^\dagger a_{i\beta} a_{i\alpha} \\
&\quad + \frac{1}{2} U_2 \sum_i \sum_{\alpha,\beta,\gamma,\delta} a_{i\alpha}^\dagger a_{i\gamma}^\dagger \mathbf{F}_{\alpha\beta} \cdot \mathbf{F}_{\gamma\delta} a_{i\delta} a_{i\beta}. \\
&= \sum_i [-\mu \hat{n}_i + \frac{1}{2} U_0 \hat{n}_i (\hat{n}_i - 1) + \frac{1}{2} U_2 (\hat{\mathbf{S}}_i^2 - 2\hat{n}_i)].
\end{aligned}
\tag{1}
$$

Here, μ and t are the chemical potential and the hopping matrix element between adjacent sites, respectively. U_0 and U_2 represent the spin-independent and the spin-dependent interactions between bosons, respectively. We assume an antiferromagnetic interaction ($U_2 > 0$). $a_{i\alpha}$ and $a_{i\alpha}^\dagger$ are the annihilation and creation operators, respectively, for a boson at site i with spin magnetic quantum number $\alpha = 1, 0, -1$. $n_i \equiv \sum_\alpha n_{i\alpha}$ ($n_{i\alpha} \equiv a_{i\alpha}^\dagger a_{i\alpha}$) is a number operator at site i. $\hat{\mathbf{S}}_i \equiv \sum_{\alpha,\beta} a_{i\alpha}^\dagger \mathbf{F}_{\alpha\beta} a_{i\beta}$ is a spin operator at site i and $\mathbf{F}_{\alpha\beta}$ represent the spin-1 matrices. $\langle i,j \rangle$ expresses a summation for all the sets of adjacent sites.

The GW of the model is defined as $\Psi \equiv \prod_i \Phi_i$. Here, Φ_i is a wave function at site i but the functional form of Φ_i is assumed to be site-independent such that $\Phi_i = \Phi$. Φ is written as a linear combination of states with N bosons at a site as $\Phi = \sum_N g(N)|N\rangle$, where $|2n+1\rangle = \sum_{S=1}^{2n+1} f(2n+1, S)|2n+1, S\rangle$ and $|2n\rangle = \sum_{S=0}^{2n} f(2n, S)|2n, S\rangle$; $|N, S\rangle$ is the state where N is the number of bosons and S is the total spin, where S must be odd for an odd and even for an even N [12]. We assume that $\hat{S}_z|N, S\rangle = 0$ [19]. Hence, Φ is an eigenstate of S_z (not S) as a quantum spin nematic state [17] in the MI state. Φ can interpolate between two limits about U_2 as $\Phi = \sum_n [g(2n)|2n, S = 0\rangle + g(2n + 1)|2n + 1, S = 1\rangle]$ ($U_2 \to \infty$) that minimizes the antiferromagnetic interaction $H_{AF} \equiv \frac{1}{2} \sum_i U_2 (\hat{\mathbf{S}}_i^2 - 2\hat{n}_i)$ and $\Phi = \sum_n g(N) a_0^{\dagger N}|0\rangle/\sqrt{N!}$ ($U_2 \to 0$) that includes high-spin states and minimizes the kinetic energy, where $|0\rangle$ is the vacuum of bosons. We note that the latter GW for $U_2 = 0$ has the same form as the GW of the spinless bosons [8]. We numerically optimize the variational parameters $g(N)$ and $f(N, S)$ to minimize the energy expectation value by Powell's method [24] under the normalization conditions $\sum_N |g(N)|^2 = 1$ and $\sum_S |f(N, S)|^2 = 1$. We select the states where the number of bosons range from $N = 0$ to $N = 6$, which are sufficient for a numerical convergence in the parameter regime studied in this paper. We define that the MI phase has a zero particle number fluctuation, and the SF phase has a finite particle
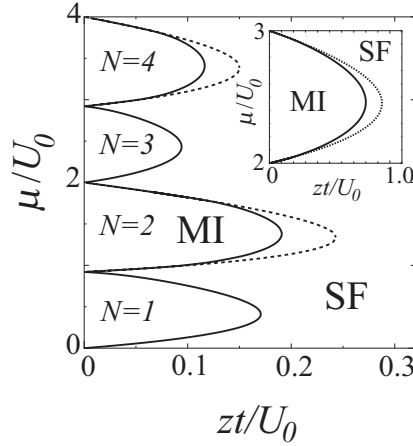
FIG. 1: Phase diagram of the Bose-Hubbard model of spin-1 bosons for $U_2/U_0 = 0.04$. Here, z is the number of adjacent sites in the lattice. SF and MI indicate the superfluid and the Mott-insulating phases, respectively. The solid and dashed curves are obtained using the GW and the PMFA, respectively. The inset indicates the SF-MI phase boundary around the MI state with $N = 3$ for $U_2/U_0 = 0.001$.

number fluctuation [20]. In an SF phase close to an MI one with N bosons, probability densities of the states for a different values of N can be considered as SF order parameters.

Figure 1 shows the phase diagram for $U_2/U_0 = 0.04$, which corresponds to ^{23}Na atoms [11]. The solid and dashed curves indicate the SF-MI phase boundaries using the GW and the PMFA, respectively. Here, z is the number of adjacent sites in the lattice. Interestingly, at a part of the phase boundary curves, the GW slightly redefines the phase boundary curves obtained using the PMFA. It will be important to note that for spinless bosons, the phase boundary obtained using the GW is the same as that obtained using the PMFA. However, an even-odd conjecture predicted in Ref. [13] still clearly holds; the MI phase with an even N is strongly stabilized against the SF phase.

On the other hand, in Fig. 1, the SF-MI phase boundary around the MI phase with an odd N obtained using the GW is the same as that obtained using the PMFA. This agreement always holds around the MI phase with $N = 1$. However, if we assume a much smaller U_2, we see a similar discrepancy between the two methods (inset of Fig. 1) around the MI phase with $N = 3$.

It should be noted that the GW including only a set of low-spin states exactly reproduces
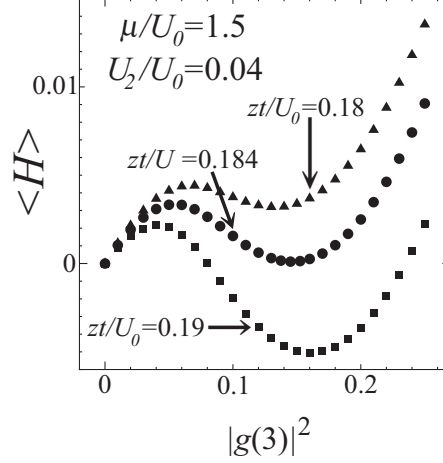
FIG. 2: Expectation values of the total energy per site $\langle H \rangle$ as a function of $|g(3)|^2$ for $U_2/U_0 = 0.04$ and $\mu/U_0 = 1.5$. The other variational parameters are determined to minimize the energy. The origin of the vertical axis corresponds to the energy of the MI state with $N = 2$. $zt = 1.9$, $zt = 1.84$, and $zt = 1.8$ correspond to an MI state, a state very close to the phase boundary, and an SF state, respectively.

the phase boundary obtained using the PMFA. For an even $N = 2n$, assuming $g(2n \pm 1) = \epsilon_{2n\pm1}$, $g(2n) = \sqrt{1 - \epsilon_{2n+1}^2 - \epsilon_{2n-1}^2}$, and $f(2n \pm 1, S = 1) = f(2n, S = 0) = 1$ ($\epsilon_{2n\pm1}$ are infinitesimal), we analytically reproduce the phase boundary curve around the Mott phase with $N = 2n$ obtained using the PMFA (Eq. 30 in Ref. [13]). We also reproduce the phase boundary obtained using the PMFA around the Mott phase with an odd $N = 2n + 1$ by numerical optimization of the GW only including the states $|2n+1, S = 1\rangle$, $|2n+2, S = 0\rangle$, $|2n + 2, S = 2\rangle$, $|2n, S = 0\rangle$, and $|2n, S = 2\rangle$. These sets of the low-spin states are nothing but the states that emerge as zero-order states or intermediate states in the second-order PMFA which determines the phase boundary [13]. This is consistent with the case of the phase boundary around the Mott state with $N = 1$ and that of spinless bosons.

In our GW, the SF phase has a polar symmetry ($\langle \mathbf{S} \rangle = 0$) and not only does the lowest spin state ($S = 1$ or $S = 0$) at a given N but also higher spin states have finite probability densities. The probability densities of the high spin states and *SF order parameters are finite just on a part of the phase boundary curve* as long as the phase boundary curve does *not* agree with that obtained using the PMFA (hereafter, we call this part of the phase boundary curve as the *non-perturbative part*). Figure 2 shows the total energy expectation value par site $\langle H \rangle$ as a function of $|g(3)|$ around a MI phase with $N = 2$, where we see
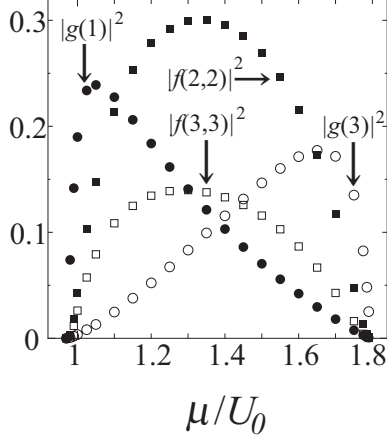
FIG. 3: Variational parameters just on the phase boundary between the SF and MI phases with $N = 2$ for $U_2/U_0 = 0.04$. The black and white circles indicate $|g(1)|^2$ and $|g(3)|^2$, respectively and the black and white squares indicate $|f(2,2)|^2$ and $|f(3,3)|^2$, respectively.

the *first-order transition* clearly. The high spin states of spin-1 bosons have an essential role in the first-order transition: for small $|g(3)|$, the PMFA calculation holds and the total energy increases with $|g(3)|$; for large $|g(3)|$, $|f(2,2)|$ and $|f(3,3)|$ become large and strongly enhance the absolute value of the kinetic energy and the total energy decreases with $|g(3)|$; for much larger $|g(3)$, the interaction energy within $|N = 3\rangle$ becomes larger and the total energy again increases with $|g(3)|$. In summation, the transition between the MI with only the lowest spin state (which has the lowest antiferromagnetic interaction energy) and the SF with higher spin states (which has a large absolute value of kinetic energy) can be a first-order one.

Figure 3 shows the chemical potential dependence of variational parameters including SF order parameters ($|g(1)|^2$ and $|g(3)|^2$) just on the phase boundary around the MI phase with $N = 2$. These parameters are found to be finite on the non-perturbative part and continuously disappear at the edges of the non-perturbative part ($\mu/U_0 \sim 0.97$ and 1.79) where the phase boundary curve agrees with that obtained using the PMFA and the transition becomes a second-order one as in the spinless case.

The phase boundary curve obtained using the GW around the MI phase with N bosons becomes close to that obtained using the PMFA for a stronger U_2 and coincide with it for a
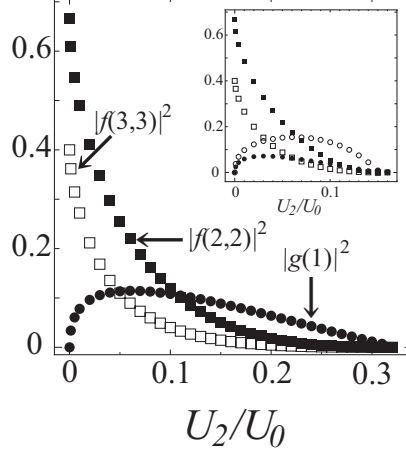
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FIG. 4: Variational parameters just on the Mott lobe of the phase boundary between the SF and MI phases with $N = 2$ as a function of U_2. The black circles indicate $|g(1)|^2$, the black and white squares indicate $|f(2,2)|^2$ and $|f(3,3)|^2$, respectively. Here, $|g(3)| = |g(1)|$ within numerical errors. The inset indicates the same variational parameters including $|g(3)|^2$ (white circles) for $\mu = 1.5/U_0$ just on the phase boundary.

finite U_2 (e.g., $U_2/U_0 \sim 0.32$ for $N = 2$ and $U_2/U_0 \sim 0.014$ for $N = 3$), where the transition becomes a second-order one along the whole phase boundary. On the other hand, for $U_2 = 0$, the transition also becomes a second-order one because the GW has the same form as that of the spinless bosons [See above (the sixth paragraph)]. Figure 4 shows the variational parameters just on the Mott lobe of the phase boundary between the SF phase and the MI phase with $N = 2$ as a function of U_2/U_0. Here, μ and zt are determined as a function of U_2 to obtain the variational parameters just at the Mott lobe. We note that the Mott lobe stays on the non-perturbative part until the phase diagram perfectly coincides with that obtained using the PMFA for $U_2/U_0 \sim 0.32$. Furthermore, $|g(3)| = |g(1)|$ holds within numerical errors. While SF order parameters $g(1)$ and $g(3)$ disappear for $U_2 = 0$ and $U_2/U_0 \sim 0.32$, $|f(2,2)|^2$ and $|f(3,3)|^2$ become larger for small U_2/U_0 and attain the maximum values for $U_2/U_0 = 0$. This is because for $U_2/U_0 = 0$, $|N = 2\rangle = a_0^{\dagger 2}|0\rangle/\sqrt{2!} = (|2,0\rangle + \sqrt{2}|2,2\rangle)/\sqrt{3}$ and $|N = 3\rangle = a_0^{\dagger 3}|0\rangle/\sqrt{3!} = (\sqrt{3}|3,1\rangle + \sqrt{2}|3,3\rangle)/\sqrt{5}$, resulting in $|f(2,2)|^2 = 2/3$ and $|f(3,3)|^2 = 2/5$. The inset of Fig.4 shows the U_2 dependence of the variational parameters for $\mu/U_0 = 1.5$ just on the phase boundary between the SF and MI phases with $N = 2$, where zt is determined to obtain the variational parameters just at the phase boundary as a function of U_2. The SF order parameters (where $|g(3)|$ is different from $g(1)$) continuously

disappear for $U_2/U_0 \sim 0.15$, where $\mu/U_0 = 1.5$ on the phase boundary appears away from the non-perturbative part.

The first-order transition may be observed in future experiments. If the lifetimes of locally stable states are sufficiently long, one can observe the first-order transition through a hysteresis curve because t/U_0 and t/U_2 can be easily controlled by the laser beam. On the other hand, the first-order transition may also be observed through the response of a spin to a weak magnetic field. The magnetization (spin expectation value) under a magnetic field may be observed by an experiment such as a Stern-Gerlach type time-of-flight measurement as discussed in Ref. [25]. We consider a uniform magnetic field parallel to the x-axis [21]. We add the Zeeman coupling $-g\mu_B B \sum_i S_{xi}$ to the Hamiltonian, where g is the Lande's g-factor of bosons, μ_B is a Bohr magneton, B is the magnetic field, and S_{xi} is the x-component of the spin at site i. We neglect the quadratic Zeeman term because a weak magnetic field of the order of mGauss or less than mGauss is sufficient [25]. In the GW, the magnetization is also site-independent such that $\langle S_{xi} \rangle = \langle S_x \rangle$. In a magnetic field, the $S_z = 0$ states are not sufficient to obtain the ground state, and hence, we employ the complete set with $S_z = -S, -S+1, \cdots, S$ in the GW. Figure 5 shows the zt/U_0 dependence of $\langle S_x \rangle$ for $U_2/U_0 = 0.04$ and $\mu/U_0 = 1.5$ under a magnetic field $g\mu_B B = 0.005$ [23]. We can clearly see that $\langle S_x \rangle$ jumps from zero to a finite value for $zt/U_0 \sim 1.85$, which corresponds to the SF-MI phase boundary under the magnetic field, and is close to that at zero magnetic field $zt/U_0 \sim 1.84$. In the MI phase, the singlet state at a site is stable under a weak magnetic field, while in the SF phase, it has a finite spin at a site resulting in a finite $\langle S_x \rangle$ under a magnetic field.[26] However, if the transition is continuous, $\langle S_x \rangle$ must be a continuous function and should not jump at the phase boundary. Hence, this jump of $\langle S_x \rangle$ is a unique result of the first-order transition.

We finally note that recent studies [17] have predicted possible nematic phases in the MI phase, while our approximation results in the lowest spin state in the MI phase regardless of the strength of $U_2(> 0)$; our study using the GW cannot include the effects of virtual hopping processes, which result in Heisenberg type spin-spin couplings between adjacent sites. However, the singlet-nematic phase boundary will be out of the MI phase in small densities of ^{23}Na atoms such as two atoms per site (the case of which is well studied in the present paper) [22]. As a matter of course, the relation and/or competition between the SF-MI transition and the singlet-nematic transition will be an interesting and open subject.
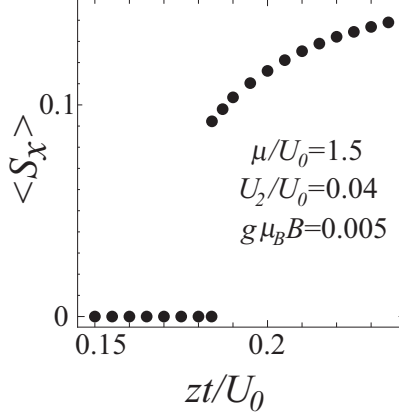
FIG. 5: zt/U_0 dependence of $\langle S_x \rangle$ for $U_2/U_0 = 0.04$ and $\mu/U_0 = 1.5$ under a magnetic field $g\mu_B B = 0.005$.

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[18] For simplicity, we neglect the weak trapping potential and assume that the system is perfectly periodic.

[19] We have numerically checked that the complete set including states with finite S_z has the same lowest energy as that of the states with only $S_z = 0$ at least within the states where the number of particles range from $N = 0$ to $N = 4$.

[20] A GW has a unique spin state in an MI because our approximation does not include inter-site effective spin coupling through virtual hopping processes [17] in the MI.

[21] Strictly speaking, the nematic axis turns in a direction perpendicular to the magnetic field to minimize the Zeeman energy when a magnetic field is applied. [For further details, see F. Zhou, Int. J. Mod. Phys. B **17**, 2643 (2003).]

[22] In refs.[17] it is suggested that the singlet-nematic transition occurs for $zt^2/(U_0 U_2) = 0.5$ in the Mott state with two bosons, which corresponds to $zt = 0.4$ for $U_2/U_0 = 0.04$ in the case of three dimensional cubic lattices with $z = 8$ (also see Fig. 1).

[23] To obtain this figure, we have employed a complete set where the number of bosons range from $N = 0$ to $N = 4$. The states with $N = 4$ have very small amplitudes ($|g(4)|^2 \lesssim 0.01$ and $|g(4)|^2/|g(3)|^2 < 0.05$), and hence, the numerical convergence is fairly sufficient.

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[26] Even if the SF phase has no total spin as a whole system (in spite of a finite spin at a site),

the magnetization will be finite under the magnetic field as long as the SF phase has no spin excitation gap.