Magnetisms of spinor alkali and alkaline atoms in optical lattices

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We theoretically investigate zero-temperature magnetic ordering of mixtures of spin-1 (alkali atoms) and spin-0 (alkaline atoms) bosons in a three-dimensional cubic optical lattice. With the single-mode approximation for the spin-1 bosons, we obtain an effective Bose-Hubbard model for describing the heteronuclear mixtures in optical lattices. By controlling the interspecies interactions between alkali and alkaline atoms, we map out complete phase diagrams of the system with both positive and negative spin-dependent interactions for spin-1 atoms, based on bosonic dynamical mean-field theory. We find that the spin-1 components feature ferromagnetic and nematic insulating phases, in addition to superfluid, depending on spin-dependent interactions. Taken the spin-1 alkali bosons as a whole (spin ↑), and spin-0 alkaline bosons as spin ↓, we observe that the system demonstrates ferromagnetic long-range order at filling \( n = 1 \), and an unordered insulator at \( n = 2 \). Interestingly, we observe a two-step Mott-insulating-superfluid phase transition, as a result of mass imbalance between alkali and alkaline atoms.

I. INTRODUCTION

Quantum magnetism plays an important role in solid state system, and many theoretical and experimental efforts have been devoted to revealing the mechanisms behind magnetic ordering of quantum many-body systems [1]. Most of studies in complex solid-state systems focus on magnetism of fermions [2], since the basic element is electron. An exception in condensed matter physics is \(^{4}\text{He}\), which is a bosonic system but its spin \( S = 0 \). Magnetism of spinful bosonic systems is exclusive, even though bosonic magnetism can enrich our understanding of many-body physics, especially about their quantum fluctuations. Therefore, it is desirable to study multi-species bosonic systems which are able to extend our understanding of quantum magnetism in many-body systems.

In the past decades, ultracold atoms trapped in periodic optical lattices have been utilized to study quantum many-body physics in a highly controllable manner [3, 4], where multi-component ultracold gases composed of fermions or bosons have been achieved [3, 4], opening new avenue for investigating quantum magnetism. Recently, an antiferromagnet has been realized in a repulsively interacting Fermi gas on a two-dimensional square lattice [7]. Two-component bosonic ultracold gases have also provided possibility for understanding quantum magnetism [8, 9], where a temperature in the order of picokelvin is achieved in a Bose-Bose mixture (pseudo-spin-1/2 Bose gases) in a three-dimensional optical lattice [8], even though the experimental temperature is still higher than the critical one of magnetic phase transition. For spin-1 bosons, the major experimental challenge is that the timescale of a spinor gas reaching ground states may exceed its lifetime, since the spin-dependent interaction (ferromagnetic or antiferromagnetic) is normally very small [10, 11].

Actually, the spinor bosonic gases lead to many interesting phenomena, including spin mixing [12], spin waves [20], spin dynamics [21], spin textures [22], and phase transitions [23, 24]. Spinor bosonic gases in optical lattices provide possibilities of entering into strongly correlated regime, and normally demonstrate two quantum phases: Mott-insulating and superfluid phases with different types of long-range magnetic order, including nematic, cyclic, ferromagnetic and antiferromagnetic long-range order [4, 22, 23]. Recently, a phase transition from a longitudinal polar phase to a broken-axisymmetry phase in condensates of spin-1 ultracold sodium atoms is demonstrated in a two-dimensional optical lattice [34], and thermal fluctuation induced stepwise Bose-Einstein condensation in a spinor gas are experimentally observed [35].

Moreover, heteronuclear mixtures of ultracold spinor bosons have been achieved experimentally, i.e., heteronuclear spinor alkali atoms [36, 37] or mixtures of spinor alkali and alkaline atoms [38–40], even though without a lattice. Different from identical spinor bosons with only even parity states being allowed for bosonic statistics, the heteronuclear mixtures of ultracold spin-1 alkali bosons in optical lattices demonstrate even richer competing many-body phases, which contains superfluid, spin-singlet, nematic, cyclic, charge-density-wave, and different types of ferromagnetic phases [39–41]. However, the magnetic phases of heteronuclear mixtures of spinor alkali and spin-0 alkaline atoms in optical lattices are still unknown.

Motivated by the experimental work [35], we investigate many-body ground states of heteronuclear mixtures of ultracold spin-1 atoms (\(^{87}\text{Rb} \) or \(^{23}\text{Na} \)) and spin-0 \(^{84}\text{Sr} \) atoms in a three-dimensional cubic optical lattice. If we treat the spin-1 alkali atoms as a whole, such as spin \( \uparrow \), and \(^{84}\text{Sr} \) as spin \( \downarrow \), we essentially achieve a pseudo-spin-1/2 bosonic model in optical lattices. Here, we focus on...
quantum magnetism of the whole system, and pay special attention to the influence of the spin-dependent interactions of spinor alkali atoms on quantum magnetism. To obtain the many-body ground states, we utilize the recently developed four-component bosonic dynamical mean-field theory (BDMFT) [42]. Similar to fermionic cases [43,44], we map the many-body lattice problem to a single-site problem which is coupled to two baths, i.e., the condensed bath and the normal bath [45,52] to take quantum fluctuations into account. In our work, complete phase diagrams of binary mixtures of ultracold spin-1 alkali and spin-0 alkaline bosons are mapped out for different interspecies interactions.

The paper is organized as follows: in section II we give a detailed derivation of the model and our approach. Section III covers our results for heteronuclear mixtures of $^{87}$Rb and $^{84}$Sr, and of $^{23}$Na and $^{84}$Sr. We summarize with a discussion in Section V.

II. MODEL AND METHOD

A. Model

We consider a heteronuclear mixture of spin-1 alkali atoms (such as $^{87}$Rb or $^{23}$Na with hyperfine spin $f = 1$) and spin-0 alkaline atoms ($^{84}$Sr with hyperfine spin $f = 0$) in a three-dimensional (3D) cubic optical lattice. For a system of identical bosonic gases with hyperfine spin $f$, the general form of the interaction can be written in the second-quantized form [53]:

$$V(x_1 - x_2) = \frac{4\pi\hbar^2}{Ma} \sum_{f=0}^{2f} a_F P_F \delta(x_1 - x_2), \quad (1)$$

where $P_F = \sum_m |F, m_F\rangle \langle F, m_F|$ is the projection operator with $|F, m_F\rangle$ being the total hyperfine spin state formed by two atoms each with spin $f$, $M_i$ the atom mass, and $a_F$ the s-wave scattering length in the channel of total spin $F$.

The interaction for homonuclear mixtures of spin $f = 1$ is given by:

$$V(x_1 - x_2) = (g_0 P_0 + g_2 P_2) \delta(x_1 - x_2)$$

where $g_0 = \frac{4\pi\hbar^2}{M_2} a_0^{(2)}$, $a_2 = \frac{4\pi\hbar^2}{M_2} a_2^{(2)}$, and $S_i$ is the spin operator of the $i$th atom with spin-1. For a heteronuclear mixture of spin-0 and spin-1 atoms, the interaction between the two-species takes the form:

$$V(x_1 - x_2) = g_{12} P_1 \delta(x_1 - x_2), \quad (3)$$

where $g_{12} = \frac{2\pi\hbar^2 a_{12}}{M_{12}}$ with the reduced mass $M_{12} = \frac{M_1 M_2}{M_1 + M_2}$. Here, $M_1$ and $M_2$ denotes the atomic mass for species 1 and 2, respectively, and $a_{12}$ the scattering length between spin-0 and spin-1 atoms. Note here that we assume the scattering lengths between spin-1 and spin-0 atoms are identical for the three-components of spin-1 atoms.

The many-body Hamiltonian for the system of heteronuclear mixtures of spin-0 and spin-1 bosonic gases takes the follow form:

$$\hat{H} = \int dx \hat{\Phi}_{m\sigma}^\dagger(x) \hat{V}(x) \hat{\Phi}_{m\sigma}(x)$$

where $\hat{\Phi}_{m\sigma}(x)$ is the field annihilation operator for the $m$ species ($m = 1$ denoting spin-1 atoms, and 2 spin-0 atoms) in the hyperfine state $\sigma = 0, \pm 1$ at point $x$, $V_{\text{lat}}$ the optical lattice potential, and $c^{(2)} = 4\pi\hbar^2 a_0^{(2)}/M_2$ with $a_0^{(2)}$ denoting the s-wave scattering length for species $m = 2$ (only one component is considered for species 2, which is denoted as $\sigma = 0$) in the total spin $s = 0$ channel.

By assuming a deep optical lattice potential and the single-mode approximation for spin-1 atoms [54], we can expand the field operator by considering only the lowest energy band $\hat{\Phi}_{m\sigma}(x) = \sum_i b_{im}\omega_m(x - x_i)$, where the Wannier function of the lowest energy band $\omega_m(x - x_i)$ is well localized in the $i$th lattice site. Following the standard derivation for ultracold bosonic gases, Eq. 4 reduces to an extended Bose-Hubbard model for heteronuclear mixtures of spin-0 and spin-1 bosons in an optical lattice, which can be written as:
\[
\hat{H} = - \sum_{\langle ij \rangle, \sigma, \sigma'} t_{m\sigma}(b_{i,m,\sigma}^\dagger b_{j,m,\sigma} + \text{H.c.}) + \sum_{i,\sigma} U_{12} b_{i,2,\sigma}^\dagger b_{i,1,\sigma} + b_{i,1,\sigma^*} b_{i,2,\sigma} \\
+ \sum_{i} \left[ \frac{1}{2} U_1 \hat{n}_{i,1}(\hat{n}_{i,1} - 1) + \frac{1}{2} U'_1 (S_{i,1}^2 - 2\hat{n}_{i,1}) + \frac{1}{2} U_2 \hat{n}_{i,2}(\hat{n}_{i,2} - 1) - \mu_1 \hat{n}_{i,1} - \mu_2 \hat{n}_{i,2} \right],
\]

where \( b_{i,m,\sigma}^\dagger \) (\( b_{i,m,\sigma} \)) is the bosonic creation (annihilation) operator for hyperfine state with \( m_F = \sigma \) for species \( m = 1, 2 \) at site \( i \), \( \hat{n}_{i,m} = \sum_{\sigma} \hat{n}_{i,m,\sigma} = b_{i,m,\sigma}^\dagger b_{i,m,\sigma} \) being the number of particles, \( S_{i,m} = \sum_{\sigma,\sigma'} b_{i,m,\sigma}^\dagger \Gamma_{\sigma\sigma'} b_{i,m,\sigma'} \) is the local spin operator with \( \Gamma_{\sigma\sigma'} \) being the usual spin matrices for a spin-1 particle, \( m_F \) denotes the chemical potential, and \( t_{m\sigma} \) the hopping amplitude on the lattice where we only consider hopping between nearest neighbors \( \langle ij \rangle \). The Hubbard repulsion \( U_1 = c_1^{(1)} \int \! dr_1 \omega_1(r - r_1)^4 \) and spin-dependent interaction \( U'_1 = c_2^{(1)} \int \! dr_1 \omega_1(r - r_1)^4 \) for spin-1 bosons, \( U_2 = c_2^{(2)} \int \! dr_2 \omega_2(r - r_1)^4 \) for spin-0 bosons, and interspecies interaction \( U_{12} = g_{12} \int \! dr \omega_1(r - r_1) \omega_2(r - r_1)^2 \) between spin-1 and spin-0 bosons. Note here that only one component is considered for species 2 with \( \sigma = 0 \).

### B. Theoretical method

To investigate quantum phenomena and obtain many-body ground states of binary mixtures of spinor alkali and alkaline Boses loaded into a three-dimensional cubic optical lattice, we utilize an extended bosonic version of dynamical mean-field theory (BDMFT) to solve the problem described by Eq. (5). The main idea of the BDMFT approach is to map the quantum lattice problem with many degrees of freedom onto a single-site problem, which is coupled self-consistently to two noninteracting baths. Here, one bath is a condensed one, and another a normal one. BDMFT treats the condensed and normal bosons on equal footing, and expands the equations up to second order as a function of \( 1/z \), where BDMFT takes the lattice coordination number \( z \) as the control parameter \( (z = 6 \) for three-dimensional cubic lattice). We remark here that BDMFT is nonperturbative, and hence can be applied within the full range from small to large couplings.

Following the standard derivation for BDMFT \([42, 40]\), we can write down the BDMFT equations in an explicit form, where the corresponding effective action of the impurity site is described by:

\[
S^{(0)}_{\text{imp}} = - \int_0^\beta \! d\tau d\tau' \sum_{m,m',\sigma,\sigma'} \left( b_{m,\sigma,\sigma'}^{(0)}(\tau) b_{m',\sigma,\sigma'}^{(0)}(\tau') \right) G^{(0)}_{\sigma\sigma'}^{-1}(\tau - \tau') \left( b_{m,\sigma,\sigma'}^{(0)}(\tau') b_{m',\sigma,\sigma'}^{(0)}(\tau) \right) + \int_0^\beta \! d\tau U_{12} n_{1,0}^{(0)}(\tau) n_{2,0}^{(0)}(\tau)
\]

\[
+ \int_0^\beta \! d\tau \left\{ \frac{1}{2} \sum_m U_m n_{m,0}^{(0)}(\tau) (n_{m,0}(\tau) - 1) + \frac{1}{2} U_1' \left[ S_1^{(0)}(\tau)^2 - 2n_{1,0}^{(0)}(\tau) \right] - \sum_{\langle ij \rangle, m, \sigma} \left( b_{m,\sigma,\sigma'}^{(0)}(\tau) \phi_{\sigma,\sigma'}(\tau) + \text{H.c.} \right) \right\}
\]

Here, \( G^{(0)}_{\sigma\sigma'}(\tau - \tau') \) is the non-interacting Weiss Green’s function:

\[
G^{(0)}_{\sigma\sigma'}^{-1}(\tau - \tau') = - \left( \partial_{\tau'} - \mu_{\sigma'} \right) \delta_{\sigma\sigma'} + t^2 \sum_{\langle i,j \rangle, \langle i,j \rangle} G^{(1)}_{\sigma\sigma',ij}(\tau, \tau') + \frac{t^2 \sum_{\langle i,j \rangle, \langle i,j \rangle} G^{(2)}_{\sigma\sigma',ij}(\tau, \tau')}{\langle \partial_{\tau'} - \mu_{\sigma'} \rangle ^2 + t^2 \sum_{\langle i,j \rangle, \langle i,j \rangle} G^{(2)}_{\sigma\sigma',ij}(\tau, \tau')}
\]

which is a \( 8 \times 8 \) matrix with \( \sigma \) running over all the possible values \( \sigma = 0, \pm 1 \) for species 1, and \( \sigma = 0 \) for species 2, to shorten the notation of Green’s functions. Here, we have defined the connected Green’s functions with the diagonal and off diagonal parts being given by:

\[
G^{(1)}_{\sigma\sigma',ij}(\tau, \tau') = - \langle b_{i,\sigma}(\tau) b_{j,\sigma'}^\dagger(\tau') \rangle_0 + \phi_{i,\sigma}(\tau) \phi_{j,\sigma'}^\dagger(\tau'),
\]

\[
G^{(2)}_{\sigma\sigma',ij}(\tau, \tau') = - \langle b_{i,\sigma}(\tau) b_{j,\sigma'}(\tau') \rangle_0 + \phi_{i,\sigma}(\tau) \phi_{j,\sigma'}(\tau'),
\]

where \( \phi_{i,\sigma}(\tau) \equiv \langle b_{i,\sigma}(\tau) \rangle_0 \) is introduced as the superfluid order parameters \( (\sigma = 0, \pm 1 \) for species 1, and \( \sigma = 0 \) for species 2), and in the cavity system \( \langle \ldots \rangle_0 \) denotes the expected value without the impurity site.

Normally, it is difficult to find an analytical solver for the effective action. To obtain many-body ground states, we turn back to the Hamiltonian representation and represent the effective action described in Eq. (6) by the
\[ \hat{H}_A^{(0)} = \sum_{m,\sigma} \left( -t_{m\sigma} \left( \phi_{m\sigma}^\dagger \hat{n}_{m\sigma} + \text{H.c.} \right) + \frac{1}{2} U_1 \hat{n}_{1\sigma}^2 - 2 \hat{n}_{1\sigma} \right) + \frac{1}{2} U_2 \hat{n}_{2\sigma}^2 - \mu_{m\sigma} \hat{n}_{m\sigma} \right) + U_{12} \hat{n}_{1\sigma}\hat{n}_{2\sigma} + \sum_{l} \varepsilon_l \hat{a}_{l\sigma}^\dagger \hat{a}_{l\sigma} + \sum_{l,m,\sigma} \left( V_{\sigma\sigma} \hat{a}_{l\sigma}^\dagger \hat{b}_{m\sigma} + W_{\sigma\sigma} \hat{a}_{l\sigma} \hat{b}_{m\sigma} + \text{H.c.} \right), \] 

where only one component is considered for species \( m = 2 \), i.e. \( \sigma = 0 \) for \( m = 2 \). Obviously, the interaction terms are identical with that in the Hubbard Hamiltonian, as in Eq. (5), since all the interactions considered here are local ones. As we mentioned above, BDMFT has reduced the many-body lattice problem to a single-site problem coupled to the condensed and normal baths, and presents equations up to subleading order. Here, the leading term is the Gutzwiller term with order parameter \( \phi_{m\sigma} \) standing for the condensed bath, and the subleading term is the normal bath described by operators \( \hat{a}_{l\sigma}^\dagger \) with energies \( \varepsilon_l \), where the coupling between the normal bath and impurity site is realized by \( V_{\sigma\sigma} \) (normal-hopping amplitudes) and \( W_{\sigma\sigma} \) (anomalous-hopping amplitudes). And then, the Anderson impurity model can be solved through numerical methods, and detailed steps have been introduced in Ref. 21, 58. Here, we use exact diagonalization as the solver to obtain the many-body ground states.

### III. RESULTS

In this paper, we investigate phase diagrams of heteronuclear mixtures of spin-1 and spin-0 atoms in a 3D optical lattice, which is characterized by the order parameter \( \phi_{m\sigma} = (b_{m\sigma}) \), magnetism \( S_1 = (\hat{b}_{1\sigma}^\dagger \Gamma_{\sigma\sigma^'} \hat{b}_{1\sigma^'}) \) for spin-1 bosons, and local total magnetism of spin-1 and spin-0 atoms \( S = \sum S_\sigma = \sum S_\sigma^0 \) with \( S_\sigma^0 \equiv (\hat{b}_{\sigma}^\dagger F_{\sigma}^0 \hat{b}_{\sigma}^\dagger) \). \sigma\ denotes the \( \sigma \)-component of species 1, and \( F_{\sigma}^0 \) is the spin matrix for a spin-1/2 particle formed by \( \sigma \)-component of species 1 and 0-component of species 2 (\( \alpha = x, y, \) and \( z \)). In our calculations, we consider the spin-miscible regime with inter-species interactions \( U_{12} < \sqrt{U_1 U_2} \), and pay special attention to the lower filling cases. We focus on both the ferromagnetic \( U_{11}^0 / U_1 < 0 \) (\( ^{87}\text{Rb} \)) and antiferromagnetic interactions \( U_{12}^0 / U_1 > 0 \) (\( ^{23}\text{Na} \)). In all our simulations, we set \( U_1 \equiv 1 \) as the unit of energy.

#### A. Mixtures of spinor \(^{87}\text{Rb} \) and \(^{84}\text{Sr} \)

We first study a mixture of spin-1 \(^{87}\text{Rb} \) and spin-0 \(^{84}\text{Sr} \) atoms in a three-dimensional optical lattice, where the Rb atoms possess a ferromagnetic interaction \( U_1^0 / U_1 = -0.0046 \) [52], and interaction between the Sr atoms \( U_2^0 / U_1 = 1.26 \) [52]. As achieved in the experiments [35, 38], the interspecies interaction between the Rb and Sr atoms \( U_{12} / U_1 \approx 0.935 \). In our simulations, we choose the hopping amplitudes \( t \approx t_{1x} \approx 0.7 \) for the four components, and chemical potential \( \mu \approx \mu_m \) for the two species.

Our results are summarized in Fig. [1] where we map out the low-filling lobes under different interspecies interactions \( U_{12} / U_1 = 0.2, 0.5, 0.935 \), and 2, obtained by bosonic dynamical mean-field theory. We observe there are four phases in the low-filling regime, including ferromagnetic phase (FM), unordered insulator (UI), two types of superfluid phases (SF). In the lower hopping regime \( t \ll U_1 \), the system demonstrates Mott-insulating phases with the spin-1 Rb atoms favoring fer-
Romagnetic spin order, which is characterized by $\phi_{\downarrow,\sigma} = 0$ and $M_1 = \langle S_1 \rangle \neq 0$, and the physical reason is that, as expected, the ferromagnetic interaction $U'_1 < 0$ supports ferromagnetic order to lower the energy of the spin-1 atoms. The results also indicate that interspecies density-density interactions between Rb and Sr do not influence the magnetic order of spin-1 bosons. We remark here that the local spin $M_t$ of the $^{87}$Rb always meet the relationship $M_t/n_{Rb} = 1$, with $n_{Rb}$ being the local total filling of $^{87}$Rb. To characterize the properties of the whole system mixed by Rb and Sr, we define the local total magnetism by taking Rb as spin $\uparrow$ and Sr as spin $\downarrow$. We find that the system possesses nonzero magnetism $M_{\text{tot}} \equiv \langle S \rangle \neq 0$ for filling $n \equiv n_{Rb} + n_{Sr} = 1$, and zero magnetism $M_{\text{tot}} = 0$ for filling $n = 2$, similar to spin-1/2 mixtures in optical lattices. Here, $n_{Sr}$ denotes the local filling of $^{84}$Sr. With the increase of the hopping amplitudes, density fluctuations dominate and superfluid phases appear with $\phi_{\downarrow,\sigma} \neq 0$. Due to the mass imbalance, the Rb atoms with larger mass delocalize first ($M_{\text{Sp}} + SF_{\text{Rb}}$), and then both species delocalize (2SF) with increasing hopping amplitudes.

Next, we study the influence of interspecies interactions $U_{12}$ on the phase diagrams. For smaller interspecies interactions with $U_{12} < \sqrt{U_1U_2}$, the two species are miscible, and the system favors phase separation for $U_{12} > \sqrt{U_1U_2}$. As shown in Fig. 1(a-d), we observe that the first lobe with filling $n = 1$ shrinks, and the second lobe with $n = 2$ expands with decreasing $U_{12}$. The physical reason is that the spins $\uparrow$ and $\downarrow$ compose a spin singlet with $M_{\text{tot}} = 0$ for $n = 2$ (as shown in Fig. 1(c), which is more favorable for smaller $U_{12}$. For a larger interspecies interaction $U_{12}/U_1 = 2$, we observe a phase separation in the system. Here, we only plot the phase diagram of spin-1 $^{87}$Rb atoms, and recover the phase diagram of spin-1 bosonic systems in optical lattice, as shown in Fig. 1(d).

For comparisons, we also investigate the mixtures of spin-1 and spin-0 bosons in optical lattices, based on Gutzwiller mean-field theory, as shown by the red lines in Fig. 1(b) (only the first Mott-insulating-superfluid transition is shown). As stated in the method part, Gutzwiller mean-field method is actually first-order approximation of BDMFT, and, by expanding to second order as a function of coordination number $z$, quantum fluctuations are taken into account and BDMFT is achieved. The phase diagrams clearly show that the tips of Mott lobe from Gutzwiller method are smaller, compared to the black lines obtained by BDMFT, as a result of quantum fluctuations which are included in BDMFT. We remark here that Gutzwiller method cannot resolve the magnetic long-rang order of Mott phases of the bosonic systems in optical lattices, since quantum magnetism is attributed to second-order tunneling processes, which are neglected in Gutzwiller static mean-field theory.

To obtain phase boundaries of the heteronuclear mixtures of spin-1 and spin-0 bosons in Fig. 1, we plot the Mott-insulating-superfluid phase transition as a function of hopping amplitudes for different chemical potentials, as shown in Fig. 2. As well known, the phase transition is filling dependent for multicomponent bosonic mixtures in optical lattices. For example, the phase transition is second order for filling $n = 1$, and can be first order for filling $n = 2$ for Bose-Bose mixtures and spin-1 bosons. The physical reason for the first-order phase transition is that the system favors a spin-singlet Mott-insulating state with even filling, which is discontinuous with the superfluid phase with nonzero magnetism, indicating a jump of spin long-range order. As shown in Fig. 2 we plot the phase transitions for chemical potentials $\mu/U_1 = 0.4$ [Fig. 2(a)], $\mu/U_1 = 1.4$ [Fig. 2(b)], and $\mu/U_1 = 1.7$ [Fig. 2(c)], which correspond to fillings $n = 1$ and $n = 2$ in the Mott-insulating regime, respectively. We clearly observe a second order phase transition from Mott insulator to superfluid for filling $n = 1$, and a first-order phase transition for filling $n = 2$ ($\mu/U_1 = 1.4$). More interestingly, we also observe a two-step phase transition at larger chemical potential ($\mu/U_1 = 1.7$), i.e., the Rb atoms delocalize first and then the Sr atoms, since...
on a special miscible case with interspecies interaction and spin-0 experimental data for heteronuclear mixtures of spinor atoms, due to the mass imbalance between Sr and Na. The other parameter are \( t \equiv t_{1\sigma} = t_{3\sigma}, U_2/U_1 = 0.66, \) and interspecies interaction \( U_{12}/U_1 = 0.4 \).

the heavier Rb atoms induce \( U_1 < U_2 \).

### B. Mixtures of spinor \(^{23}\)Na and \(^{84}\)Sr

In contrast to the results that we mentioned above, in this section we focus on the mixtures of spin-1 \(^{23}\)Na and spin-0 \(^{84}\)Sr in a 3D optical lattice. Different from spin-1 \(^{87}\)Rb, the spin-dependent interaction here is an antiferromagnetic one for \(^{23}\)Na with \( U_1/U_1 = 0.037, U_2/U_1 = 0.66 \). As far as we know, there are no experimental data for heteronuclear mixtures of spinor \(^{23}\)Na and spin-0 \(^{84}\)Sr, and, without loss of generality, we focus on a special miscible case with interspecies interaction \( U_{12}/U_1 = 0.4 \).

For the spin-1 bosons \(^{23}\)Na with antiferromagnetic interactions, the spin-1 bosons favor different types of spin long-range order in the Mott-insulating region depending on the local filling. For example, the spin-1 bosons in optical lattices demonstrate spin nematic order for odd filling, characterized by \( \phi_{1\sigma} = 0, \varphi_{1_{\alpha\beta}} = \langle S_{1\alpha}S_{1\beta} \rangle - \delta_{\alpha\beta} \cdot \langle S_{1\beta}^2 \rangle > 0 \) and \( M_1 = 1 \), and spin-singlet order for even filling, characterized by \( \phi_{1\sigma} = 0, \varphi_{1_{\alpha\beta}} = 0 \) and \( M_1 = 0 \), with \( \alpha \) being one of the three-components of spin-1 bosons. Here, by mixing the spin-1 antiferromagnetic bosons with spin-0 closed-shell bosons in optical lattices, we observe there are four phases in the low-filling regime, including ferromagnetic phase (FM), unorder insulator (UI), two kinds of superfluid phases (SF), as shown in Fig. 3. Similar to the ferromagnetic case, such as \(^{87}\)Rb, the interspecies interactions between Na and Sr do not influence the spin long-range order of spin-1 bosons in the parameters studied here, i.e. the spin-1 bosons favor spin nematic order both for filling \( n = 1 (n_{23Na} = 0.5) \) and for \( n = 2 (n_{23Na} = 1) \). The physical reason is that the spin-1 bosons favor nematic spin order for filling \( n_{23Na} \) being odd. We also examine the local total magnetism of the whole system mixed by \(^{23}\)Na and \(^{84}\)Sr in optical lattices, and find that the system favors nonzero magnetism for filling \( n = 1 \) (FM) and zero magnetism for \( n = 2 \) (UI) in the Mott-insulating regime.

With increasing hopping amplitudes, density fluctuations dominate and the system demonstrates a phase transition from the Mott insulator to the superfluid phase, as shown in Fig. 4. As expected, we observe a second-order Mott-insulating-superfluid transition for filling \( n = 1 \). Similar to the mixture of Rb and Sr, we also observe a two-step Mott-insulating-superfluid phase transition at higher filling, i.e. the Sr atoms delocalize first, and then the Na atoms, which is a result of the mass imbalance between the Na and Sr atoms. Note here that the spin-1 \(^{23}\)Na atoms support a nematic-insulating-polar-superfluid phase transition both for local total filling \( n = 1 \) and 2, which is different from the situation with only the spin-1 bosons loaded into optical lattices for even fillings.

### IV. CONCLUSIONS

In conclusion, we have investigated quantum phases of binary mixtures of spin-1 alkali and spin-0 alkaline bosons loaded into a cubic optical lattice, based on recently developed four-component bosonic dynamical mean-field theory. Complete phase diagrams both with ferromagnetic and antiferromagnetic interactions are obtained. Interestingly, we find that the system demonstrates nonzero magnetic long-range order and a second-order Mott-insulating-superfluid phase transition for filling \( n = 1 \), and a first-order phase transition for \( n = 3 \).
2. In addition, we observe a two-step Mott-insulating-superfluid phase transition, as a result of mass imbalance between alkali and alkaline atoms. We expect the spontaneous spin long-range order of heteronuclear mixtures in optical lattices can be realized and detected using current experimental techniques.

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