Spin-1 Bose-Hubbard model with two- and three-body interactions

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We investigated the ground state of spin-1 bosons interacting under local two- and three-body interactions in one dimension by means of the density matrix renormalization group method. We found that the even-odd asymmetry will be obtained or not depending on the relative values of the two- and three-body interactions. The Mott insulator lobes are spin isotropic, the first showing a dimerized pattern and the second being composed of singlets. The three-body interactions disfavor a longitudinal polar superfluid and a quantum phase transition to a transverse polar superfluid occurs, which could be continuous or discontinuous.

I. INTRODUCTION

The macroscopic occupation of a unique quantum state was observed by confining alkalai atoms with magneto-optical traps, opening a new branch of the physics called ultracold atoms, which has linked and promoted several areas of physics [1]. The possibility of exploring diverse physical phenomena led to the development of new cooling and trapping techniques, in particular new ways to confine atoms without freezing the spin degree of freedom, which was achieved by creating purely optical traps with lasers [2]. Using the above technique to confine sodium or rubidium atoms, it has been possible to observe a Bose-Einstein condensate for each hyperfine state [3]. Larmor precession [4], spin dynamics [5], coherent spin dynamics [6], and spontaneous symmetry breaking [7], among other phenomena. Note that cold-atom setups constitute a new means of studying quantum magnetism [8] and the interplay between charge and spin degrees of freedom [9].

Cold-atom setups are highly tunable, allowing the experimental observation of a reversible quantum phase transition between a superfluid state and a Mott insulator one for bosonic atoms in magneto-optical traps by Greiner et al. [10]. To observe the transition, one needs to efficiently control the ratio of interactions to the mobility of atoms by increasing the depth of an optical lattice, manipulating interactions with Feshbach resonance [11], or periodically shaking the lattice [12]. The superfluid-Mott insulator transition for spinless bosons is second-order and has been described in terms of the Bose-Hubbard Model [33–36] and the emergence of new proposals where multi-body interactions are considered in spinless boson systems [37, 38]. To understand the experimental results, taking into account multi-body interactions in spinless boson chains [33–36] and the emergence of new proposals where the three-body interactions are dominant [37, 38].

Confining $^{87}$Rb atoms in optical lattices, it was possible to observe evidence of the effects of multi-body interactions using an atom interferometric technique [31] or photon-assisted tunneling experiments [32]. This experimental evidence of multi-body interactions stimulated several theoretical studies on the effect of taking into account multi-body interactions in spinless boson chains [33–36] and the emergence of new proposals where the three-body interactions are dominant [37, 38]. To understand the experimental results, taking into account the spin degree of freedom, Mahmud and Tiesinga made a calculation using perturbation theory and derived effective spin-dependent and spin-independent three-body interaction potentials [39]. Recently, the ground state of a spinor gas under only three-body interactions was studied numerically, finding that the even-odd asymmetry of the two-body antiferromagnetic chain is absent and the density drives first-order superfluid-Mott insulator transitions for even and odd lobes [40].
The phase diagram of spin-1 bosons under two- and three-body interactions was calculated by Nabi and Basu using mean-field theory [41]. They found that as the area of the Mott lobes increases with respect to the superfluid region, the critical point of the superfluid-Mott insulator transition moves to larger values of the hopping with the strength of the three-body interaction term, and they concluded that for antiferromagnetic interactions, the even-odd asymmetry remains. Motivated by these results, we decided to take a step beyond the mean-field and study the S-1 Bose-Hubbard Hamiltonian with two- and three-body interactions using the density matrix renormalization group method. We found that for the parameters of Nabi and Basu the even-odd asymmetry does not occur, and this is retained for larger values of the two-body spin-dependent interaction. We also observed a quantum phase transition from a longitudinal polar superfluid to a transverse polar superfluid due to the three-body interactions.

The rest of the article is organized as follows: In Sec. II we set up the spin-1 Bose-Hubbard model with two- and three-body interactions, and the atomic limit is considered. We present our main numerical results in Sec. III based on the density matrix renormalization group method. We summarize our results in Sec. IV.

II. MODEL

Taking into account the interaction terms between spin-1 bosons proposed by Imambekov et al. [17] and Mahmud et al. [39], a degenerate gas of spin-1 atoms can be described by the following effective Hamiltonian

\[ H = -t \sum_{i,\sigma} \left( b_{i,\sigma}^\dagger b_{i+1,\sigma} + h.c. \right) + \sum_{i} \left\{ n_i (\tilde{n}_i - 1) - \frac{U_0}{2} + \frac{V_0}{2} (\tilde{n}_i - 2) \right\} + \sum_{i} \left\{ (\tilde{S}_i^2 - 2\tilde{n}_i) \right\} , \]

where \( b_{i,\sigma}^\dagger \) creates (annihilates) a boson with spin component \( \sigma \) on site \( i \) of a one-dimensional optical lattice of size \( L \), the total number of particles at the site \( i \) is \( \tilde{n}_i = \sum_{\sigma} n_{i,\sigma} \) and \( n_{i,\sigma} = b_{i,\sigma}^\dagger b_{i,\sigma} \). Representing the spin-1 Pauli matrices by \( T_{\sigma,\sigma'} \), the local spin operator is \( \tilde{S}_i = \sum_{\sigma,\sigma'} b_{i,\sigma}^\dagger T_{\sigma,\sigma'} b_{i,\sigma'} \).

The physical meaning of each term in the Hamiltonian (1) is: The first term describes the kinetic energy of bosons with \( t \) being the tunneling force between nearest sites. The interactions between bosons appear in the remaining terms; specifically, the spin-independent terms and the spin-dependent interactions are shown in the second and third line, respectively. The parameter \( U_s \) represents the two-body interaction in the \( S \) channel given by \( U_0 = 4\pi \hbar^2 (a_0 + 2a_2) / 3M \) and \( U_2 = 4\pi \hbar^2 (a_2 - a_0) / 3M \) where \( a_s \) are the scattering lengths for \( S = 0 \) and \( S = 2 \) channels and \( M \) is the mass of the atom [2]. In the present paper, we consider \( U_2 > 0 \), i.e. antiferromagnetic interaction. The three-body interaction parameters are \( V_0 \) and \( V_2 \). The validity of the perturbation theory imposes \( V_0 << U_0 \) and \( V_2 = 2U_2 / V_0 [39] \).

At the atomic limit of the Hamiltonian (1) \(( t \to 0)\), the energy is given by

\[ E_M(n_e) = n_e (n_e - 1) \left[ \frac{U_0}{2} + \frac{V_0}{6} (n_e - 2) \right] + \left( < \tilde{S}_i^2 > - 2n_e \right) \left[ \frac{U_2}{2} + \frac{V_2}{6} (n_e - 2) \right] , \]

while for an odd number of particles \(( n_o \) \)

\[ E_M(n_o) = n_o (n_o - 1) \left[ \frac{U_0}{2} + \frac{V_0}{6} (n_o - 2) \right] + (1 - n_o) \left[ U_2 + \frac{V_2}{3} (n_o - 2) \right] . \]

The absence of the kinetic term leads to a ground state with an integer number of interacting particles per site; hence the ground state is a Mott insulator one. The boundaries of the Mott lobes at the atomic limit are given by \( \mu(n \to n + 1) = E(n + 1) - E(n) \), which corresponds to the chemical potential under the canonical ensemble. Taking into account the above definition, we obtain \( \mu(n_o \to n_o + 1) = U_0 n_o - 2U_2 + \frac{V_0}{6} n_o - V_2 (1 - n_o) \) and \( \mu(n_e \to n_e + 1) = U_0 n_e + \frac{V_0}{6} n_e - V_2 (1 - n_e) \). From the above expressions, we found that for a finite nonzero \( V_0 \) value, the odd lobes decrease as the two-body spin interaction parameter \(( U_2 \) \) grows, and note that these lobes do not vanish when \( U_2 \) reaches its maximum value \( U_2 / U_0 = 0.5 \). Also, the upper boundary of the Mott lobes with even filling is independent of \( U_2 \). Now, if we fix \( U_2 \), we obtain that the boundaries of the first Mott lobe are independent of the three-body interactions, a fact that we expected, because we do not have fluctuations. As we increase the density, the three-body spin-independent interaction parameter has an important role in increasing the area of the Mott lobes.
III. NUMERICAL RESULTS

As the hopping parameter is turned on ($t \neq 0$), the particles can be delocalized, and quantum fluctuations emerge in the system. Due to this, the ground state will change, and we expect a ground state with delocalized particles, when the kinetic energy will be the dominant energy scale. Therefore, the Hamiltonian exhibits different ground states, and we need to distinguish between the diverse phases of the model. A first option is to calculate the charge gap at the thermodynamic limit. For finite lattices of size $L$, the charge gap is given by $\Delta(L) = \mu^0(L) - \mu^0(L) = E_0(L, S^z, N+1) + E_0(L, S^z, N-1) - 2E_0(L, S^z, N)$ where $\mu^0(L)$ is the chemical potential to add (remove) a particle, and $E_0(L, S^z, N)$ is the ground state energy of a lattice with $N$ spin-1 bosons and $S^z$ projection of the total spin. We use the density matrix renormalization group (DMRG) method with open boundary conditions to calculate the ground state for lattices of a size up to $L = 128$. The dimension of the local Hilbert space basis is fixed by choosing a maximum occupation number $\hat{n}_{\text{max}} = 5$ to guarantee accurate results. In the DMRG procedure, we kept up to $m = 350$ states per block and obtained a discarded weight around $10^{-5}$ in the worst case, and the ground-state energy converges to an absolute error of $10^{-3}$ or better. We set our energy scale choosing $U_0 = 1.0$ and studied the ground-state for various values of the interacting parameters considering that $U_2 < 0.5U_0$, $V_0 << U_0$ and $V_2 = 2\sqrt{t/U_0}$.

We took into account the theorems proposed by Katsura et al., and all the calculations presented in this paper were done in the sector with $S^z = 0$.

The evolution of the ground state as the number of particles increases is shown in Fig. 1 for a finite chain with $L = 28$ sites, a fixed hopping $t/U_0 = 0.10$, and interaction parameters $U_2/U_0 = 0.05$, $V_0/U_0 = 0.10$, and $V_2/U_0 = 0.01$. The above parameters were chosen taking into account a recent mean-field calculation about spinor bosons with two- and three-body interactions. We observe that the chemical potential increases monotonously as the global density grows, but at integer densities a plateau appears, which indicates that a finite energy gap was found for integer densities and the ground state corresponds to an incompressible Mott insulator at the thermodynamic limit. Far away from the integer densities, we do not obtain an energy gap. Therefore, the ground state is compressible and the spinor bosons are delocalized throughout the lattice. We found that the ground state can be either superfluid or Mott insulator. Note that the length of the plateau for the global density $\rho = N/L = 2$ is larger than the one for $\rho = 1$, which is due to two-body spin-interaction. From Fig. 1, it is clear that the compressibility $\kappa = \partial \rho / \partial \mu$ is always positive, a fact that suggests the absence of first-order phase transitions from superfluid to Mott insulator.

In 2009, Batrouni et al. reported a first-order transition at the second lobe of a spinor systems with only two-body interactions in spite of $\kappa = \partial \rho / \partial \mu > 0$ [30, 45]. For a spinor chain under only three-body interactions, we showed that the phase transitions are of the first-order kind for even and odd Mott lobes [40]. In order to explore what happens in a one-dimensional system of spin-1 bosons under two- and three-body interactions, we calculated the spin population fraction in each spin projection $(N_+/N$ and $N_0/N)$. The component $N_-/N$ is not necessary due to $N_+/N = N_0/N$ as a function of the global density, and the results are shown in Fig. 2. Taking into account that the wave function of a singlet state is $|2,0\rangle = \sqrt{2/3}|1,-1\rangle|1,1\rangle - \sqrt{1/3}|1,0\rangle|1,0\rangle$; in this

FIG. 1. Global density $\rho$ as a function of the chemical potential $\mu$ for a finite chain of $L = 28$ sites. The plateau indicates the possibility that for integer densities Mott insulator phases occur. Two different superfluid regions appear: longitudinal polar superfluid (LPS) and transverse polar superfluid (TPS). The parameters here are $t/U_0 = 0.10$, $U_2/U_0 = 0.05$, $V_0/U_0 = 0.10$, and $V_2/U_0 = 0.01$. The lines are visual guides.

FIG. 2. The spin population fraction in each spin projection $(N_+/N$ and $N_0/N$) and the $z$-component of the nematic order parameter $Q_{zz}$ as a function of the global density $\rho$ for a finite chain of $L = 28$ sites, a fixed hopping $t/U_0 = 0.10$ and interaction parameters $U_2/U_0 = 0.05$, $V_0/U_0 = 0.10$, and $V_2/U_0 = 0.01$. The lines are visual guides.
state, we must obtain that \( N_+ / N = N_- / N = N_0 / N \), which happens in the range \( 1.5 \lesssim \rho \lesssim 2.1 \). However, for densities different from \( \rho = 2 \), singlets bound states of two spinor bosons try to form themselves for a finite lattice, this being exactly achieved at the thermodynamic limit only with \( \rho = 2 \). These results are similar to those reported by Batrouni et al. However, as the density increases, we observe a quantum phase transition from a longitudinal polar superfluid \((N_0 > N_+)\) to a transverse polar superfluid \((N_0 < N_+)\), which happens due to the three-body interactions between the spin-1 bosons. Comparing these results with our previous report about spinor bosons with only three-body interactions \([40]\), we observe that the critical density for which the quantum transition from longitudinal polar to transverse polar superfluid occurs will depend on the two- and three-body interactions.

In order to characterize the magnetic order in spin-1 systems, it is important to calculate the \( z \)-component of the nematic order parameter \( Q_{zz} = \langle \hat{S}_z^2 \rangle - \frac{1}{3} \langle \hat{S}_z^3 \rangle \), because in our case \( Q_{xx} = Q_{yy} \). Then we obtain on-site spin isotropy if \( Q_{zz} = 0 \) and spin anisotropy if \( Q_{zz} \neq 0 \), which is characteristic of the nematic order \([43, 46]\). In Fig. 2, we see that the \( z \)-component of the nematic order parameter vanishes for global densities \( \rho \leq 2 \); hence for the hopping parameter \( t / U_0 = 0.10 \), the Mott insulator and superfluid regions will not be nematic. A longitudinal polar superfluid is characterized by the predominant \( \sigma = 0 \) spin population \((N_0 > N_+)\) and this is spin isotropic \( Q_{zz} = 0 \). The ground state remains a longitudinal polar superfluid for densities slightly greater than \( \rho = 2 \), and then the \( z \)-component of the nematic order parameter jumps to a finite value, which coincides with the change in the spin population fractions, now \( Q_{zz} \neq 0 \) and a non-nematic to nematic quantum phase transition has occurred. A transverse polar superfluid is characterized by the predominant \( \sigma = \pm 1 \) spin population.
FIG. 5. The square of the local moment \( <S^2> \) as a function of the hopping parameter \( t/U_0 \) for a global density \( \rho = 2 \). Here, we consider a chain with \( L = 28 \) sites, and the interaction parameters are \( U_2/U_0 = 0.05 \), \( V_0/U_0 = 0.1 \), and \( V_2/U_0 = 0.01 \). Inset: The same as the main plot but for \( \rho = 1 \). The vertical dashed line indicates the position of the Mott insulator-superfluid transition, which corresponds to \( t_c/U_0 = 0.28 \) and \( t_c/U_0 = 0.185 \) for the first and the second Mott lobe, respectively. The lines are visual guides.

\((N_+ > N_0)\), and it is spin anisotropic \( Q_{zz} \neq 0 \). Our numerical results indicate that the quantum phase transition from a longitudinal polar superfluid to a transverse polar superfluid is discontinuous. Note that a discontinuous phase transition between two superfluid phases for \( ^7 \)Li atoms in a three-dimensional optical lattice was discussed recently, but in this case the transition is driven by a quadratic Zeeman term, which competes with the ferromagnetic interaction between the spin-1 bosons [17].

In Fig. 3 we show the dependence of the system size on the chemical potential of a chain of spinor bosons with global density \( \rho = 1 \) and interaction parameters \( U_2/U_0 = 0.05 \), \( V_0/U_0 = 0.1 \), and \( V_2/U_0 = 0.01 \). The upper set of data shows the energy needed to add a particle to the system, while the lower one the energy needed to remove a particle, which were obtained with DMRG. The values at the thermodynamic limit \( (N, L \to \infty) \) were calculated by extrapolation, considering quadratic or linear dependence. The left panel shows the results for \( t/U_0 = 0.10 \) (Fig. 3a), while the right one shows the results for \( t/U_0 = 0.28 \) (Fig. 3b), and it is evident that the ground state changes as the hopping parameter increases. We obtain a gapped state for small values of the hopping with an integer number of particles per site; hence the ground state is a Mott insulator one, but as the hopping grows, we expect that spinor bosons will delocalize throughout the lattice and the ground state will be gapless (superfluid). This figure shows us that a quantum phase transition from a superfluid state to a Mott insulator one will take place as the hopping parameter decreases as the two- and three-body interactions between spinor bosons are considered. The above conclusion is expected when we are studying interacting bosons; however, the most interesting problem is related to the phase diagram, for which recent mean-field studies suggest that the even-odd asymmetry always happens [11].

Although physical arguments and mean-field calculations lead to the conclusion that the ground state of interacting spinless or spinor bosons may be either Mott insulator or superfluid, with the superfluid surrounding the Mott insulator lobes, an accurate determination of the boundaries between these phases is an interesting problem that has been considered in many papers by means of different approaches and techniques. For instance, an accurate phase diagram for spinor bosons in one dimension with two-body (three-body) interactions between them was found using numerical approaches (DMRG and/or QMC) [22, 30] (Fig. 4). We used the DMRG algorithm to find the phase diagram of a chain of spinor bosons under two- and three-body interactions by calculating the chemical potential to add or remove one particle at the thermodynamic limit for different values of the hopping, when the parameters \( U_2, V_0 << U_0 \), and \( V_2 = 2/t_0 V_0 \) are fixed. Mean-field phase diagrams for this problem were recently reported by Nabi and Basu [41], and we show them in Fig. 4a and Fig. 4b (Rounded green and yellow regions, respectively). Note that the mean-field results suggest that the even-odd asymmetry of spinor bosons with two-body interactions is maintained with three-body interactions. We found that the extrapolated values from the DMRG results at the atomic limit are in agreement with the mean-field calculations and with our previous analysis; therefore, borders of the Mott lobes depend on the interaction parameters \( U_2 \) and \( V_0 \). In Fig. 4c, the interaction parameters are \( U_2/U_0 = 0.05 \), \( V_0/U_0 = 0.1 \), and \( V_2/U_0 = 0.01 \), and we obtained that for very small values of \( t/U_0 \), the mean-field and the results from DMRG data are close, but as the value of \( t/U_0 \)
increases, the mean-field lobes close quickly, whereas the numerical ones close very slowly, moving the critical point to larger values of the hopping, and giving to the lobes an elongated shape regardless the global density. Note that the odd lobes are larger than the even lobe, indicating that the even-odd asymmetry suggested by the mean-field calculation is an artifact of the method, and that the three-body interactions contribute more to the localization of the particles for global densities greater than $\rho = 1$. The first lobe remains almost the same, while the others grow, especially the Mott lobe with $\rho = 3$, whose critical point is higher than the one for $\rho = 2$. Maintaining the same spin-dependent two-body interaction value $U_2/U_0 = 0.05$ but increasing the spin-independent three-body interaction value $V_0/U_0 = 0.5$, we obtain the phase diagram shown in Fig. 4. There, the borders of the first Mott lobe do not change at the atomic limit, and due to the small fluctuations of charge, the three-body interactions are of little importance, leading to a first Mott lobe similar to the one in the previous figure, but with a slightly lower critical value. For the second lobe, we see that at the atomic limit the gap depends on the parameter $V_0$ and the three-body interactions become more important due to the increase in the global density, leading to the growth of second Mott lobe and to its critical point’s moving to larger values of the hopping. Something similar happens for the third Mott lobe, this being the largest lobe for these parameters, with a critical point at $t_c(\rho = 3) \approx 0.32U_0$. Hence we conclude that for a fixed two-body spin interaction, the three-body interactions increase the Mott lobes for densities greater than $\rho = 1$, and their critical points move to larger values of the hopping.

Up to now, we have considered the spin two-body interaction equal to $U_2/U_0 = 0.05$ due to the phase diagrams reported by Nabi and Basu. However, the above value is small. Taking into account this fact, we consider a larger value $U_2/U_0 = 0.30$ and draw the phase diagram shown in Fig. 4 for $V_0/U_0 = 0.1$ and $V_2/U_0 = 0.06$. This time the odd Mott lobes are very small and the even one predominates in the phase diagram, showing the well-known even-odd asymmetry characteristic of spinor chains with only two-body interactions; i.e. for larger spin two-body interactions and smaller three-body interactions, the even-odd asymmetry is preserved. Comparing Fig. 4 with the results reported by Rizzi et al. [22] for only two-body interactions, we observe that the first lobe is almost the same and the second one has a larger gap at the atomic limit, but the critical point is similar. At the atomic limit, the gap of the Mott lobe for $\rho = 3$ is reduced by the interactions. The lower border rises due to $V_0/U_0$, while the upper border lowers due to $U_2/U_0$, but the smaller three-body interactions become important, elongating the lobe until it reaches a higher critical point $t_c(\rho = 3) \approx 0.24U_0$, which is higher than the case with only two-body interactions. Again, if we set the spin two-body interaction and increase the three-body interactions, the Mott lobes for $\rho > 1$ grow and their critical points go to larger values (not shown).

Using different approaches and/or numerical techniques, several authors have shown that the magnetic properties of superfluid and Mott insulator phases of spin-1 boson systems are diverse and interesting. For instance, for an antiferromagnetic chain with two-body interactions, it has been suggested that the even Mott lobes exhibit a singlet and a nematic phase, whereas the odd lobes exhibit a dimerized phase [22, 30]. When only three-body interactions are considered, it has been shown that the ground state is not composed of singlets at the second Mott lobe [10]. The formation or lack thereof of singlets at the Mott lobes can be shown by calculating the square of the local moment ($< S^2 >$), as shown in Fig. 3 for a chain with $L = 28$ sites, $U_2/U_0 = 0.05$, $V_0/U_0 = 0.1$, and $V_2/U_0 = 0.01$. For one spinor boson per site ($\rho = 1$), we note that $< S^2 >$ is finite and nonzero in both the Mott and the superfluid regions (see inset of Fig. 3). Obviously, no local singlets are formed, and the well-known dimerized pattern for this filling is obtained (not shown).

Increasing the global density up to $\rho = 2$, we observe that $< S^2 >$ is non-zero for larger values of the hopping in the superfluid region. However, as the hopping decreases, $< S^2 >$ decreases monotonously, both in the superfluid region and in the Mott insulator lobe, reaching zero value at the atomic limit, where we have a singlet at each site. Note that the transition point shown in Fig. 3 corresponds to a naive estimation based on the vanishing of the charge gap, which is not valid when a first-order transition takes place, as in the superfluid-Mott insulator transition for $\rho = 2$.

For a fixed global density $\rho = 2$ (main plot) and $\rho = 1$ (inset), the evolution of the $z$-component of the nematic order parameter $Q_{zz}$ versus the hopping parameter is shown in Fig. 6 from deep in the Mott lobes to the superfluid phase. We found that in the Mott insulator lobes, the spin remains isotropic: $Q_{zz} = 0$. This re-

![FIG. 7. The nematic structure factor $Q_{zz}$ as a function of the global density $\rho$ at the superfluid region. Here the parameters are $t/U_0 = 0.30$, $U_2/U_0 = 0.05$, $V_0/U_0 = 0.1$ and $V_2/U_0 = 0.01$. The lines are visual guides.](image-url)
sult is expected for $\rho = 1$, because the ground state is dimerized; however, for $\rho = 2$, our finding is curious, because the possibility of a singlet-nematic transition in even lobes has been suggested by several authors [31, 42]. Our ground state is composed of singlets, and the $< S^2 >$ non-zero values are due to the quantum fluctuations. The inset of Fig. 6 tells us that the ground state is not nematic for either the Mott insulator or the superfluid regions when one boson per site is considered, but for a global density $\rho = 2$, the ground state is not nematic in the Mott lobe, but shortly after the transition the spin anisotropy ($Q_{zz} \neq 0$) grows continuously starting at zero in the superfluid region, this being a behavior similar to that reported in 2D for larger values of the two-body spin dependent interaction [42]. In the superfluid region and at $t/U_0 = 0.30$, we see that the ground state is non-nematic and nematic for densities $\rho = 1$ and $\rho = 2$, respectively. Due to this fact, we calculated $Q_{zz}$ as a function of the global density in the superfluid region, and the results are shown in Fig. 7. We obtained that the ground state is a longitudinal polar superfluid for small densities, but for densities larger than $\rho \approx 0.55$, a continuous quantum phase transition takes place and the ground state becomes a transverse polar superfluid except for $\rho = 1$, for which the ground state is always a longitudinal polar superfluid. Note that the evolution of the spin anisotropy is monotonous except for the integer densities, for which it falls. Recently, direct experimental evidence of spin-nematic ordering in a spin-1 Bose-Einstein condensate of sodium atoms with antiferromagnetic interactions has been shown. We believe that based on these measurements it could be possible to identify multi-body interaction effects [48].

IV. CONCLUSIONS

To summarize, in the present paper, we used the density matrix renormalization group to study the ground state of spin-1 bosons loaded into a one-dimensional optical lattice interacting via two- and three-body spin dependent and independent interaction terms, considering only antiferromagnetic interaction. The ground state can be Mott insulator or superfluid, and the border between them was found for different sets of the interaction parameters, showing that the well-known even-odd asymmetry for the case with only two-body interactions does not obtain and depends on the relative values of the two- and three-body interactions, contradicting the mean-field results of Nabi and Basu, who suggested that the even-odd asymmetry persists [11]. We found that the three-body interactions do not alter the kind of transition, i.e. the first (second) Mott insulator-superfluid transition is second- (first-) order. Regardless of the strength of the two-body spin-dependent interactions, between the second and the third Mott lobe a quantum phase transition from a longitudinal polar superfluid to a transverse polar superfluid takes place. Exploring the magnetic properties of the first two Mott lobes, we found that they are spin isotropic, the second Mott lobe being composed of singlets, preventing the possibility of a nematic phase inside, which has been suggested for the case with only two-body interactions in one and two dimensions. For one boson per site the superfluid is always longitudinal. Our numerical results suggest that the longitudinal-transverse polar superfluid transition can be either continuous or discontinuous, and the critical density for which it happens decreases as the hopping parameter increases, in a way similar to quantum transitions between superfluid states in a spinor system with a quadratic Zeeman potential [47].

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[1] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
[2] D. M. Stamper-Kurn and M. Ueda, Rev. Mod. Phys. 85, 1191 (2013).
[3] D. M. Stamper-Kurn, M. R. Andrews, A. P. Chikkatur, S. Inouye, H.-J. Miesner, J. Stenger, and W. Ketterle, Phys. Rev. Lett. 80, 2027 (1998).
[4] J. M. Higbie, L. E. Sadler, S. Inouye, A. P. Chikkatur, S. R. Leslie, K. L. Moore, V. Savalli, and D. M. Stamper-Kurn, Phys. Rev. Lett. 95, 050401 (2005).
[5] J. Stenger, S. Inouye, D. M. Stamper-Kurn, H.-J. Miesner, A. P. Chikkatur, and W. Ketterle, Nature 396, 345 (1998).
[6] M.-S. Chang, Q. Qin, W. Zhang, L. You, and M. S. Chapman, Nat. Phys. 1, 111 (2005).
[7] L. E. Sadler, J. M. Higbie, S. R. Leslie, M. Vengalattore, and D. M. Stamper-Kurn, Nature 443, 312 (2006).
[8] D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, and T. Esslinger, Science 340, 1307 (2013).
[9] A. V. Gorshkov, M. Hermle, V. Gurarrie, C. Xu, P. S. Julienne, J. Ye, P. Zoller, E. Demler, M. D. Lukin, and A. M. Rey, Nat. Phys. 6, 289 (2010).
[10] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature 415, 39 (2002).
[11] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, Rev. Mod. Phys. 82, 1225 (2010).
[12] H. Lignier, C. Sias, D. Ciampini, Y. Singh, A. Zenesini, O. Morsch, and E. Arimondo, Phys. Rev. Lett. 99, 220403 (2007).
[13] T. D. Kühner and H. Monien, Phys. Rev. B 58, R14741(R) (1998).
[14] S. Ejima, H. Fehske, and F. Gebhard, Europhys. Lett. 93, 30002 (2011).
[15] T. Kimura, S. Tsuchiya, and S. Kurihara, Phys. Rev. Lett. 94, 110403 (2005).
[16] J. Jiang, L. Zhao, S.-T. Wang, Z. Chen, T. Tang, L.-M. Duan, and Y. Liu, Phys. Rev. A 93, 063607 (2016).
[17] A. Imambekov, M. Lukin, and E. Demler, Phys. Rev. A 68, 063602 (2003).
[18] M. Theis, G. Thalhammer, K. Winkler, M. Hellwig, G. Ruff, R. Grimm, and J. H. Denschlag, Phys. Rev. Lett. 93, 123001 (2004); G. Thalhammer, M. Theis, K. Winkler, R. Grimm, and J. H. Denschlag, Phys. Rev. A 71, 033403 (2005).
[19] S. K. Yip, Phys. Rev. Lett. 90, 250402 (2003).
[20] A. Imambekov, M. Lukin, and E. Demler, Phys. Rev. Lett. 93, 120405 (2004).
[21] S. Tsuchiya, S. Kurihara, and T. Kimura, Phys. Rev. A 70, 043628 (2004).
[22] M. Rizzi, D. Rossini, G. D. Chiara, S. Montangero, and R. Fazio, Phys. Rev. Lett. 95, 240404 (2005).
[23] S. Bergkvist, I. P. McCulloch, and A. Rosengren, Phys. Rev. A 74, 053419 (2006).
[24] V. Apaja and O. F. Syljuasen, Phys. Rev. A 74, 035601 (2006).
[25] R. V. Pai, K. Sheshadri, and R. Pandit, Phys. Rev. B 77, 014503 (2008).
[26] Y. Toga, H. Tsuchiura, M. Yamashita, K. Inaba, and H. Yokoyama, J. Phys. Soc. Jpn. 81, 063001 (2012).
[27] T. Kimura, Phys. Rev. A 87, 043624 (2013).
[28] S. S. Natu, J. H. Pixley, and S. D. Sarma, Phys. Rev. B 91, 043620 (2015).
[29] Y. Li, L. He, and W. Hofstetter, Phys. Rev. A 93, 033622 (2016).
[30] G. G. Batrouni, V. G. Rousseau, and R. T. Scalettar, Phys. Rev. Lett. 102, 140402 (2009).
[31] S. Will, T. Best, U. Schneider, L. Hackermüller, D.-S. Lühmann, and I. Bloch, Nature 465, 197 (2010).
[32] R. Ma, M. E. Tai, P. M. Preiss, W. S. Bakr, J. Simon, and M. Greiner, Phys. Rev. Lett. 107, 095301 (2011).
[33] J. Silva-Valencia and A. M. C. Souza, Phys. Rev. A 84, 065601 (2011).
[34] J. Silva-Valencia and A. M. C. Souza, Eur. Phys. J. B 85, 161 (2012).
[35] T. Sowinski, Phys. Rev. A 85, 065601 (2012).
[36] S. Ejima, F. Lange, H. Fehske, F. Gebhard, and K. Müster, Phys. Rev. A 88, 063625 (2013).
[37] A. J. Daley and J. Simon, Phys. Rev. A 89, 053619 (2014).
[38] S. Paul, P. R. Johnson, and E. Tiesinga, Phys. Rev. A 93, 043616 (2016).
[39] K. W. Mahmud and E. Tiesinga, Phys. Rev. A 88, 023602 (2013).
[40] A. F. Hincapie-F. R. Franco, and J. Silva-Valencia, Phys. Rev. A 94, 033623 (2016).
[41] S. S. Nabi and S. Basu, ArXiv:1606.02897v2 (2016).
[42] S. R. White, Phys. Rev. Lett. 69, 2863 (1992).
[43] H. Katsura and H. Tasaki, Phys. Rev. Lett. 110, 130405 (2013).
[44] G. G. Batrouni, and R. T. Scalettar, Phys. Rev. Lett. 84, 1599 (2000).
[45] L. de Forges de Parny, F. Herbert, V. G. Rousseau, and G. G. Batrouni, Phys. Rev. B 88, 104509 (2013).
[46] E. Demler and F. Zhou, Phys. Rev. Lett. 88, 163001 (2002).
[47] K. H. Z. So and M. Ueda, ArXiv:1604.01163v3 (2016).
[48] T. Zibold, V. Corre, C. Frapolli, A. Invernizzi, J. Dalibard, and F. Gerbier, Phys. Rev. A 93, 023614 (2016).