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Quantum entanglement of spin-1 bosons with coupled ground states in optical lattices

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Abstract

We examine particle entanglement, characterized by pseudo-spin squeezing, of spin-1 bosonic atoms with coupled ground states in a one-dimensional optical lattice. Both the superfluid and Mott-insulator phases are investigated separately for ferromagnetic and antiferromagnetic interactions. Mode entanglement is also discussed in the Mott-insulating phase. The role of a small but nonzero angle between the polarization vectors of counter-propagating lasers forming the optical lattice on quantum correlations is investigated as well.

1. Introduction

The investigation of atomic bosons with short-range repulsive interactions in a periodic potential using the Bose–Hubbard model has revealed a quantum phase transition between two distinct phases: a superfluid and a Mott insulator, that exists at sufficiently low temperatures [1]. The formalism of the Bose–Hubbard model was successfully mapped onto a system of cold bosonic atoms in an optical lattice [2]. The superfluid to Mott-insulator phase transition was experimentally realized [3] and further examined and theoretically digested [4]. Continued progress has focused on systems of multi-component Bose–Einstein condensates (BECs) in an optical lattice [5], where diverse topics such as quantum phase transitions of spin-2 bosons [6], two-component condensates [7], and spin-1 bosons with coupled ground states [8] have been studied.

An interesting feature characterizing a variety of lattice models mapped onto atomic gases is quantum entanglement. Additionally, cold-atom-based lattice models have been identified as ideal candidates for universal quantum emulation of strongly interacting many-body systems. While a complete understanding of quantum entanglement and correlations in an atomic lattice model remains a significant challenge even in theoretical terms [18], much has been understood for an important type of correlation, the so-called spin squeezing, or pseudo-spin squeezing. For those systems that undergo quantum phase transitions, the presence and the measure of entanglement are important not only at the transition point, but also for the different phases of the system. These systems show various behaviours, entanglement and disentanglement, coherent and squeezed spin states, mode and particle entanglement for different phases that can be controlled by interaction types and strengths as well as lattice configurations.

Squeezed spin states are states whose spin fluctuation in one of the transverse spin components is below the standard quantum limit. It was shown in [19] a spin-s squeezed spin state is a correlated state consisting of $2s$ spin-1/2 particles. This implies a potential connection between spin squeezing and entanglement, due to the existence of correlations affecting the separability of a system with many spin-1/2 particles [20]. Spin squeezing can occur in many models with a variety of atom–atom interactions [21, 22], for atomic condensates inside external traps [20], and for atoms inside optical lattices [23].

In this work, we are interested in the possibility and the condition for spin squeezing in the pseudo-spin of coupled ground states in an optical lattice model with spin-1 bosons. We hope to explore spin squeezing properties of the system carefully studied in [8]. This paper is organized as follows. In section 2, we review the model system [8, 24] and describe the mapped Bose–Hubbard Hamiltonian in the mean-field approximation. The measure of spin squeezing and quantum

entanglement that we employ is introduced in section 3. The results of spin squeezing for different interaction regimes are presented in section 4. Finally, we conclude in section 5.

2. Model system

The system we study consists of neutral bosonic atoms with hyperfine spin $F = 1$ in an optical lattice. The optical lattice results from the ac Stark shifts of standing wave laser fields, which are dipole coupled to atomic electronic transitions. The off-resonant coupling induces virtual transitions to electronic excited states, which upon adiabatic elimination give rise to level shifts (ac Stark shifts) in the ground-state manifold. These shifts are proportional to the intensity distribution of the laser light. Additionally two-photon Raman-like transitions can couple any two Zeeman states within the spin-1 ground-state manifold, subject to appropriate polarization selections. In a lattice of ac Stark shifts from standing waves, the periodic level shift gives rise to band structures. When the lasers are linearly polarized, the Zeeman ground-state manifold of $(M_F = -1, 0, +1)$ remains degenerate in the lattice. For more general cases of coupling referred to as the Λ or V scheme with suitable polarizations, two alternate ground states become coupled and will be denoted as the electronic modes with $\sigma = 0$ and $\sigma = \Lambda$ [8].

We assume that atoms will remain in the lowest Bloch bands as a result of the relatively large band gap in comparison with their kinetic energies. Within this approximation, the atomic field operator can be expanded in terms of the site localized Wannier basis. As carefully presented in [8], we arrive at the model Hamiltonian defined on a 1D optical lattice as given below,

$$
\begin{aligned}
\hat{H}_{\text{BH}} = & -\sum_{\sigma=0,\Lambda} |J_\sigma| \sum_{\langle i,j \rangle} \hat{a}^\dagger_{\sigma i} \hat{a}_{\sigma j} \\
& + \sum_{\sigma=0,\Lambda} \frac{U_\sigma}{2} \sum_i \hat{n}_{\sigma i}(\hat{n}_{\sigma i} - 1) + K \sum_i \hat{n}_{0i} \hat{n}_{\Lambda i} \\
& - \frac{|P|}{2} \sum_i \left(\hat{a}^\dagger_{0i} \hat{a}^\dagger_{0i} \hat{a}_{\Lambda i} \hat{a}_{\Lambda i} + \hat{a}^\dagger_{\Lambda i} \hat{a}^\dagger_{\Lambda i} \hat{a}_{0i} \hat{a}_{0i} \right) \\
& - \delta \sum_i \hat{n}_{0i} - \mu \sum_{\sigma=0,\Lambda} \sum_i \hat{n}_{\sigma i},
\end{aligned} \tag{1}
$$

where J_σ is the tunnelling parameter, U_σ, K and P are parameters from the repulsive density–density interaction of condensed atoms and the spin-exchange interaction. δ parameterizes the energy difference between the electronic internal states $\sigma = 0$ and $\sigma = \Lambda$. μ is the chemical potential, $\hat{a}^\dagger_{\sigma i}$ and $\hat{a}_{\sigma i}$ are respectively creation and annihilation operators of an atom in mode σ at lattice site i and $\hat{n}_{\sigma i} = \hat{a}^\dagger_{\sigma i} \hat{a}_{\sigma i}$.

As discussed in [8], the various parameters of the above Hamiltonian (1) can be given in terms of Wannier spinors, and thus they depend on θ, the angle between the polarization vectors of the two counter-propagating linearly polarized laser beams in the lin-θ-lin configuration of an optical lattice.

In the mean-field approximation [25] with $\psi_\sigma = \langle \hat{a}_{\sigma j} \rangle$ assumed real [8], we substitute

$$
\hat{a}^\dagger_{\sigma i} \hat{a}_{\sigma j} \approx \psi_\sigma \left(\hat{a}_{\sigma j} + \hat{a}^\dagger_{\sigma i} \right) - \psi_\sigma^2, \tag{2}
$$

into the Hamiltonian (1), and arrive at

$$
\begin{aligned}
\hat{H}_{\text{BH}}^{\text{MF}} = & -2 \sum_{\sigma=0,\Lambda} J_\sigma \left[\left(\hat{a}_\sigma + \hat{a}^\dagger_\sigma \right) \psi_\sigma - \psi_\sigma^2 \right] \\
& + \sum_{\sigma=0,\Lambda} \frac{U_\sigma}{2} \hat{n}_\sigma (\hat{n}_\sigma - 1) \\
& + K \hat{n}_0 \hat{n}_\Lambda - \frac{|P|}{2} \left(\hat{a}^\dagger_0 \hat{a}^\dagger_0 \hat{a}_\Lambda \hat{a}_\Lambda + \hat{a}^\dagger_\Lambda \hat{a}^\dagger_\Lambda \hat{a}_0 \hat{a}_0 \right) \\
& - \delta \hat{n}_0 - \mu \sum_{\sigma=0,\Lambda} \hat{n}_\sigma, \tag{3}
\end{aligned}
$$

a system of many independent sites. In the above, we have omitted the site index i so that effectively, the optical lattice model is reduced to a collection of single site problems.

The basic idea of mean-field theory (MFT) is to replace the fluctuating exchange field by an effective average field in an interacting many-body system. MFT has been found not quite reliable to describe critical phenomena especially at low dimensions [9]. In MFT, one ignores the long-range fluctuations of the order parameter which causes serious errors at the critical points where the fluctuations dominate the mean value [10]. Despite these facts, optical lattices have extensively been studied under an MFT approach [2, 11]. The interaction term in the Bose–Hubbard model for the optical lattices, e.g. the interaction terms in (1), is due to atom–atom collisions which can happen only locally, so that it is an on-site interaction. The sole non-local interaction is the hopping term, due to tunnelling of the atom between the sites. As in the case of our spin-1 model, MFT treats the spin–spin interactions exactly while the kinetic coupling is treated approximately.

MFT, as it is used here, based upon the Bogoluibov symmetry breaking background field theory. Bogoluibov theory is extended to describe Mott transition by a specific decorrelation approximation in a consistent MFT [12]. It can be systematically improved by considering bigger clusters (two sites or more) to employ MFT [13]. Away from phase boundaries such an improvement is not essential for us. The fluctuations are due to collective excitations of the system. Focusing at zero temperature, and staying away from the phase boundaries, one can expect that the predicted MFT ground states are well established, since the collective excitations and associated fluctuations would be weaker in comparison to the mean-field order parameter. In our investigations we assume that the reported ground states [8] describe the system in deep quantum phases away from the phase boundaries.

A similar approach, as is done here, to determine the ground states has been employed in a more general system that includes external magnetic field as well [14]. MFT cannot be used to examine spin–spin correlations among different sites for which effective models can be used [15]. On site spin fluctuations however can be examined in MFT to reveal any particle entanglement associated with the reported ground states [8]. The question we address here is how the type and amount of the entanglement among the particles in a single lattice site would change when the whole lattice system undergoes quantum phase transitions and the use of MFT is sufficient for this question.

Beyond zero-temperature, a generalization of the method is given in [16]. At non-zero temperatures it is more crucial to

test predictions of MFT for low-dimensional systems against numerical tests. For spin-1 systems, detailed numerical studies became only very recently available [17]; but they have ensured that similar level of agreement between the MFT predictions and numerical studies as in spinless systems do occur for the case of spin-1 systems.

In order to test the validity of MFT that we use in our model, we studied a simple lattice model having two sites. We used the Bose–Hubbard Hamiltonian in (1) and *i* runs from 1 to 2 with the periodic boundary conditions. The purpose of this calculation is to investigate the effect of inter-site interaction on the single-site state. The exact ground-state calculations were done by using those parameter values corresponding to $n = 1$ and $n = 2$ Mott phases in the phase diagrams both for the ferromagnetic and antiferromagnetic regimes in the case of $\theta = 0$ and for a small θ value. Once the exact two-site ground state is determined, we calculate the one-site density matrix by tracing out the other site. Following this procedure, the overlap of ground states from MFT and exact two-site model can be computed. Our results show that most of these overlap values are above 0.95, confirming the success of MFT in calculating one-site ground states and the use of it to quantify correlations among particles in a single site.

In general, many-body wavefunctions are too complicated to express explicitly, but MFT allows for writing analytical wavefunctions of the ground states and hence one can gain valuable insights into the quantum correlations in such complex many-body systems such as spinor condensates in optical lattices. This insight should serve as a guide even for comprehending quantum correlations among the lattice sites which require beyond MFT calculations, but can still be performed through perturbative examinations of mean-field ground states. We hope to investigate this in the near future.

A general spin-1 system is described by the symmetry group SU(3). In the model considered here, a reduced two-mode description for the two coupled ground states is represented by a pseudo-spin-1/2 algebra, effectively the isospin subgroup of SU(3) [8]. The corresponding generators of the SU(2) isospin algebra are given by [8]

$$
\begin{aligned}
\hat{T}_1 &= \frac{1}{2}\big(\hat{a}_\Lambda^\dagger \hat{a}_0 + \hat{a}_0^\dagger \hat{a}_\Lambda\big), \\
\hat{T}_2 &= \frac{\mathrm{i}}{2}\big(\hat{a}_\Lambda^\dagger \hat{a}_0 - \hat{a}_0^\dagger \hat{a}_\Lambda\big), \\
\hat{T}_3 &= \frac{1}{2}\big(\hat{a}_0^\dagger \hat{a}_0 - \hat{a}_\Lambda^\dagger \hat{a}_\Lambda\big),
\end{aligned}
\tag{4}
$$

in terms of which the mean-field Hamiltonian (3) can be expressed as

$$
\begin{aligned}
\hat{H}_{\mathrm{BH}}^{\mathrm{MF}} &= -2\sum_{\sigma=0,\Lambda} J_\sigma\big[\big(\hat{a}_\sigma + \hat{a}_\sigma^\dagger\big)\psi_\sigma - \psi_\sigma^2\big] \\
&\quad + \frac{U_\Sigma}{2}\hat{T}_3^2 + (K - |P|)\hat{T}_1^2 + (K + |P|)\hat{T}_2^2 \\
&\quad + \frac{U_\Sigma}{8}\hat{n}^2 - \left(\frac{K}{2} + \mu + \frac{U_\Sigma}{4} + \frac{\delta}{2}\right)\hat{n} \\
&\quad - \left(\frac{\Delta U}{2} + \delta\right)\hat{T}_3 + \frac{\Delta U}{2}\hat{n}\hat{T}_3,
\end{aligned}
\tag{5}
$$

where $\Delta U = U_0 - U_\Lambda$, $U_\Sigma = U_0 + U_\Lambda$ and $\hat{n} = \hat{n}_0 + \hat{n}_\Lambda$. Spin-dependent interaction terms in this Hamiltonian emulates that of the generalized Lipkin–Meshkov–Glick (LMG) model [26, 27], or its special case of the two-axis twisting model [19]. Such models are capable of generating spin squeezing [19] and multiparticle entanglement [21, 26]. Our model above includes tunnelling and collision effects in addition to the generalized LMG interaction terms.

When the lattice parameter $\theta = 0$, the two modes have the same energy and $J_0 = J_\Lambda = J$, $U_0 = U_\Lambda = U$, $K = U + P$ and $\delta = 0$ [8]. The simplified Hamiltonian (3) takes the following form

$$
\begin{aligned}
\hat{\mathcal{H}}_{\mathrm{af(f)}} &= -2J\sum_{\sigma=0,\Lambda}\big[\big(\hat{a}_\sigma^\dagger + \hat{a}_\sigma\big)\psi_\sigma - \psi_\sigma^2\big] \\
&\quad + 2\big(U\hat{T}^2 + P\hat{T}_{2(1)}^2\big) + \alpha\hat{n},
\end{aligned}
\tag{6}
$$

for both antiferromagnetic ($P > 0$) and ferromagnetic ($P < 0$) interactions [24], where we have used $\hat{T}^2 = \hat{n}^2/4 + \hat{n}/2$ for the collision interaction in terms of the total isospin operator $\hat{T}^2$ with $\alpha = -3U/2 - P/2 - \mu$. The spin interaction now reduces to that of a single-axis twisting type [19].

The above considerations show that our model allows for the investigation of effects due to tunnelling and collision on spin squeezing induced by either the two-axis twisting interaction as in the generalized LMG model or the single-axis twisting interaction in the simplified case. In the general case of the LMG model, particle entanglement thus exists for atoms in the non-degenerate ground-state modes, which become degenerate for the special case of a lattice with $\theta = 0$.

3. Spin squeezing and quantum entanglement

Squeezed spin states defined by Kitagawa and Ueda [19] are widely used in atomic physics, especially in the context of particle correlation and entanglement. A criterion was found recently connecting many-atom entanglement and correlation originally from atoms in a Bose–Einstein condensate (BEC) [20]. If the squeezing parameter

$$
\xi_\alpha^2 = \frac{N(\Delta J_\alpha)^2}{\langle J_\beta\rangle^2 + \langle J_\gamma\rangle^2},
\tag{7}
$$

is smaller than 1, the two-mode bosonic many-atom state under consideration is spin squeezed along the direction of α. $\vec{J}$ is the total pseudo-spin operator, while α, β and γ denote three orthogonal axes. The condition for $\xi_\alpha^2 < 1$ coincides with the non-separability criterion of a density matrix for N two-state boson [20]. Thus ξ_α^2 can be used to measure quantum entanglement in the two-state atomic system discussed above. In our study outlined below, we examine spin squeezing for the on-site isospin algebra by calculating the variance and expectation values of the corresponding generators T_i defined in (4). Our results show clearly the existence of quantum correlations between atoms on the same lattice site.

To identify pairwise entanglement in our many-body system, we can make use of a direct relationship between concurrence [28], which is well-known and represents a widely accepted measure of bipartite entanglement, and spin squeezing criterion [29]. Thus, we take (7) as an indicator for

two-particle entanglement. We will in addition also calculate the concurrence and compare the results with the squeezing parameter (7).

In view of the significant difficulties of measuring spin squeezing along any arbitrary direction α, our investigation will focus on the simplest case of a single orthogonal configuration with three fixed axes. Other orthogonal axes configurations may be sequentially searched for if the optimal squeezing is to be found. For this aim we only need to rotate the coordinate system about each of the axes by an angle ϕ. For example if the rotation is about the axis-3, ξ_3^2 remains the same, while the squeezing parameters for the new axis-1 and axis-2 become

$$\xi_{1'}^2 = N \frac{\Delta T_1^2 \cos^2\phi + \Delta T_2^2 \sin^2\phi - \sin\phi\cos\phi\langle T_1, T_2\rangle}{\langle T_3\rangle^2 + (\langle T_1\rangle \sin\phi + \langle T_2\rangle \cos\phi)^2},$$

$$\xi_{2'}^2 = N \frac{\Delta T_1^2 \sin^2\phi + \Delta T_2^2 \cos^2\phi + \sin\phi\cos\phi\langle T_1, T_2\rangle}{\langle T_3\rangle^2 + (\langle T_1\rangle \cos\phi - \langle T_2\rangle \sin\phi)^2}, \quad (8)$$

where $\langle T_i, T_j\rangle = \langle T_i T_j + T_j T_i\rangle - 2\langle T_i\rangle\langle T_j\rangle$.

4. Results

4.1. Numerical method

The mean-field Bose–Hubbard Hamiltonian in (3) has been used to examine the phase transition between the superfluid and Mott-insulator phases [8], with ψ_σ denoting the order parameter for the σ mode. The superfluid phase for the σ component is identified with $\psi_\sigma \neq 0$. In the superfluid state the tunnelling term J_σ is large and dominates the Hamiltonian. As a result the ground state corresponds to the single-particle wavefunction of all σ-type atoms extended over the whole lattice, with each site being a coherent superposition of Fock number states [3]. In the Mott phase, on the other hand, the interaction term dominates so that the ground state exhibits minimal number fluctuation and corresponds to a product of atom Fock number states at each lattice site, which in turn gives $\psi_\sigma = 0$ [3].

We have performed numerical diagonalization of the mean-field Hamiltonian (3) by using a set of states expanded in terms of the product of individual atom number states

$$|\Omega\rangle = \sum_{n_0=0}^{N} \sum_{n_\Lambda=0}^{N} c_{n_0 n_\Lambda} |n_0\rangle |n_\Lambda\rangle. \quad (9)$$

While performing this diagonalization, two different regimes with respect to the same parameter P must be carried out. One is for a positive antisymmetric coupling, with a corresponding antiferromagnetic ground state, where individual spins are anti-aligned due to spin-exchange interaction. The other case is ferromagnetic for a negative spin exchange interaction. In addition, we explore the dependence of our results on the small, but non-vanishing lattice parameter θ, which introduces a spin-dependent lattice potential.

We study the parameter regions corresponding to those considered in [8]. The values of the parameters in Hamiltonian (3), which are needed for numerical computation, are thus read from figure 1 of [8], with J/U chosen to ensure the system has full access to the $n = 2$ Mott regime, but barely
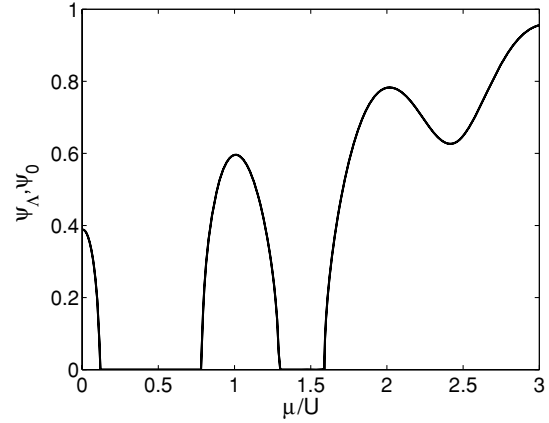

Figure 1. The dependence of the order parameters on the value of μ/U for $\theta = 0$, $J/U = 0.455 \times 10^{-1}$ and $P/U = -0.926 \times 10^{-2}$ in the ferromagnetic regime. The vanishing of the order parameters matches closely with the appearance of Mott-insulator phases for the corresponding component.

enters the $n = 3$ Mott phase. θ is taken to be small and δ values used are for the range of $0 \leqslant \theta \leqslant 1$. We study the degenerate ($\theta = 0$) and non-degenerate cases ($\theta \neq 0$) separately. From the initial values of the order parameters ψ_0 and ψ_Λ we compute the diagonal basis and the corresponding ground state. This ground state then allows us to calculate the new order parameters and to compare with the initial values. This procedure is iterated to reach a self-consistent solution, with which it becomes straightforward to calculate the expectation values and the second moments of the operators in (4).

To conveniently calculate the squeezing parameter ξ^2 (7), we use the average total occupation number $\langle \hat{n}\rangle$ for each type of interactions to label the different phases instead of relying on the total number of atoms N (per site). This implicitly assumes that the squeezing parameter (7) remains a valid criterion of quantum entanglement even for non-integer occupation numbers such as in the superfluid phase. This assumption does not introduce any inconvenience in a Mott phase since the ground state consists of Fock states with equal total number of particles, i.e., definite spin and thus $\langle \hat{n}\rangle$ becomes an integer. In the superfluid phase, we justify the use of a non-integer $\langle \hat{n}\rangle$ in the following manner. In this section, we calculate the squeezing parameter in two different ways for each case. The first method uses $\langle \hat{n}\rangle$ directly for the entanglement measure. The second method is analogous in form, but only uses integer values of $\langle \hat{n}\rangle$. For the superfluid phase, instead of talking about separability for states with different total number of particles, we focus on the subspace $n_0 + n_\Lambda = n$ block and investigate its correlation. This becomes a meaningful measure when the block we use is the one with the nearest integer total number of particles to $\langle \hat{n}\rangle$. This method has a similar nature as the superselection rules mentioned in [18] and in [30] since the projection of the Hilbert space onto a subspace of fixed particle number is considered. Both methods are found to give similar behaviours for the superfluid and the Mott-insulator phases. We provide results from the first method in our discussion because they respect the collective nature of the superfluid state and emphasize particle number fluctuations.

There also exist states for which spin squeezing parameter cannot be readily used to characterize their correlation properties. An example is the maximally entangled states (MES) in [31], which are not squeezed spin states according to the criterion in (7). In this case, it is inadequate to talk about squeezing, since the uncertainty in the perpendicular components to the mean isospin vector are meaningless as the denominator for the squeezing measure (7) vanishes for all axes. In addition, there exist other states, although whose averaged mean isospin are nonzero, the expectation values for the two components in the denominator might vanish, also making the spin squeezing parameter ξ_i^2 not well defined. In our studies, we find that these states happen only in certain Mott phases, where exact wavefunctions are available either analytically in the spin [24] or Fock basis [8]. As such, their quantum entanglement properties can be discussed directly using other criteria.

In order to quantify the pairwise quantum correlations both in the superfluid and Mott-insulator regimes, in addition to the squeezing parameter, we use the well-known criterion called concurrence [28]. For a given two-party state ρ, this measure is equal to

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{10}$$

where λ_i's are the square roots of the eigenvalues of $\rho\tilde{\rho}$ in decreasing order where

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y). \tag{11}$$

For the $n = 1$ Mott-insulator phase, this measure is trivial since there is only one particle present. When it comes to the $n = 2$ Mott phase, concurrence clearly quantifies pairwise correlations between the two atoms at the same lattice site. In the superfluid phase, the ground state is a superposition of Fock states with different number of atoms or isospin states with different isospins, we again focus on the subspace with the nearest integer total number of particles $n_0 + n_\Lambda = n$. If the nearest integer is smaller than 2, then concurrence is zero. If it is equal to 2, the concurrence is simply calculated. When it is equal to 3, the three-particle ground state is symmetrized in the first quantization picture and we use reduced two-body density matrix to calculate concurrence.

We report below our investigation of quantum entanglement in our model system for the two regimes: antiferromagnetic and ferromagnetic interactions.

4.2. Ferromagnetic regime

For ferromagnetic interaction with $P < 0$, for $\theta = 0$, and a fixed J/U value, the dependence of the order parameters ψ_0 and ψ_Λ on the quantity μ/U is shown in figure 1. We determine the phase of the system for any μ/U value by looking at the order parameter of each component.

Quantum correlations on a single lattice site is evidenced by evaluating the squeezing parameter (7). In the superfluid regime, numerical calculations, taking into account the minimization with respect to coordinate rotations, yield $\xi_i^2 > 1$. So there is no particle entanglement in the superfluid phase of a ferromagnetically interacting system when $\theta = 0$. However, this situation deserves to be more carefully analysed

for those values of μ/U that correspond to Mott-insulator phases.

The spin squeezing parameter is not defined for the zero particle ($n = 0$) ground state $|0, 0\rangle$, the trivial case of no particle entanglement without any particles. When $\theta = 0$, the single particle ($n = 1$) ground states $|10\rangle$ and $|01\rangle$ are degenerate [8] and can be written as $|g\rangle = \cos x|01\rangle + \sin x \exp(iy)|10\rangle$, where $x, y \in [0, 2\pi]$ are arbitrary angles, parameterizing the manifold of the ground-state family. We find $\langle T_1 \rangle = (1/2)\sin 2x \cos y$, $\langle T_2 \rangle = (-1/2)\sin 2x \sin y$, and $\langle T_3 \rangle = (-1/2)\cos 2x$. The spin fluctuations are $\langle \Delta T_1^2 \rangle = (1/4)(1 - \sin^2 2x \cos^2 y)$, $\langle \Delta T_2^2 \rangle = (1/4)(1 - \sin^2 2x \sin^2 y)$ and $\langle \Delta T_3^2 \rangle = (1/4)(\sin^2 2x)$. Thus we obtain $\xi_i^2 = 1$ in any direction $i = 1, 2, 3$, for any member of the ground-state manifold. The ground state, expressed in the spin representation [24], could be written as an arbitrary superposition of $|T = 1/2, T_1 = \pm 1/2\rangle$ spin states. We write $|g\rangle = |x, y\rangle = \cos(x/2)|1/2, 1/2\rangle + \sin(x/2)\exp(iy)|1/2, -1/2\rangle$ for the ground state in spin representation. Projection of the total spin onto the (x, y) direction gives the spin component $S_{x,y} = \sin x \cos y T_2 + \sin x \sin y T_3 + \cos x T_1$, whose eigenstate is $|x, y\rangle$ with eigenvalue $1/2$, such that $S_{x,y}|x, y\rangle = (1/2)|x, y\rangle$. Such a state is called a coherent spin state (CSS) [19]. The ground state $|g\rangle$ is identified as a pure state of a spin-1/2 system, and as such is a CSS. There exists no other spin to be correlated with, so that $|g\rangle$ cannot be a squeezed spin state (SSS). Particles in a CSS are correlated as all spin-1/2 constituents atoms are pointing along the same direction; although they remain separable, i.e., they are not entangled.

On the other hand, the $n = 1$ Mott state could become mode entangled [32] for some α and β. Mode entanglement is a different concept from particle entanglement considered here and could be useful for different applications [32]. It corresponds to entanglement in the second quantization picture, while particle entanglement is associated with the inseparability of the wavefunction, or density matrix, in the first quantization.

Similarly, the ground states for the $n = 2$ Mott phase are also degenerate for $\theta = 0$. As such they form a manifold represented by $|g\rangle = \cos x|11\rangle + \sin x \exp(iy)|b\rangle$, where $|b\rangle = (|02\rangle + |20\rangle)/\sqrt{2}$. In this case, $\langle T_1 \rangle = \sin 2x \cos y$ and $\langle T_{2,3} \rangle = 0$. The variances are calculated to be $\langle \Delta T_1^2 \rangle = 1 - \sin^2 2x \cos^2 y$, $\langle \Delta T_2^2 \rangle = \cos^2 x$, and $\langle \Delta T_3^2 \rangle = \sin^2 x$. ξ_1^2 becomes either undetermined (a 0/0 form) or ∞ due to vanishing denominators. If we calculate ξ_1^2 after a coordinate rotation by ϕ about the axis-3, we find $\xi_{1'}^2$. Minimizing it with respect to ϕ, we finally get $(\xi_{1'}^2)_{\min} = 1/(2\sin^2 x \cos^2 y)$ with its minimum value at $\phi = \pm\pi/2$. We find $\xi_3^2 = 1/(2\cos^2 x \cos^2 y)$ and $\xi_2^2 = 1/(2\sin^2 x \cos^2 y)$. For some values of x and y, $\xi_{2,3}^2 < 1$ is satisfied. Hence, particle entanglement exists for some members of the ground-state manifold. This is consistent with the fact that each degenerate ground state $|11\rangle$ and $|b\rangle$ is particle entangled. For parameters x and y specifying a dominant contribution from a particular degenerate component in $|g\rangle$, particle entanglement is expected. In the spin representation, the ground state is an arbitrary superposition of $|T = 1, T_1 = \pm 1, 0\rangle$. In contrast to
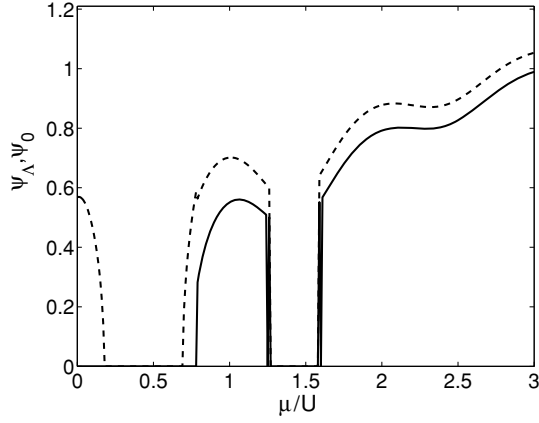
Figure 2. The dependence of order parameters for the two modes versus μ/U for a small nonzero θ in the ferromagnetic regime with $J/U = 0.625 \times 10^{-1}$, $P/U = -0.926 \times 10^{-2}$ and $\delta/U = 0.327 \times 10^{-2}$. The solid line denotes ψ_Λ while the dashed line refers to ψ_0.

Figure 3. The dependence of the order parameters on the values of μ/U for $\theta = 0$ in the antiferromagnetic regime with $J/U = 0.455 \times 10^{-1}$ and $P/U = 0.926 \times 10^{-2}$. The nonzero valued order parameters indicate superfluid phases for the corresponding components.

the spin-1/2 case of the $n = 1$ Mott phase, now squeezed spin state (SSS), where all particles are entangled, can be found in the ground-state family.

When we analyse ferromagnetic regime by calculating the concurrence in light of the discussion in section 4.1, it is found to be zero for all μ/U values except those for the $n = 2$ Mott phase. In this case, the ground state is an arbitrary superposition of two degenerate maximally entangled states, with the concurrence for each state being equal to one. But the concurrence for the ground-state manifold mentioned above becomes $C(|g\rangle) = [1 - (1/2)\sin^2(2x)\cos(2y)]^{1/2}$, which is larger than zero for some values of x and y. And this indicates the possibility of pairwise entanglement for certain ground states.

Now we look at the situation when θ takes a small but nonzero value. In this case the relations $J_0 \approx J_\Lambda = J$, $U_0 \approx U_\Lambda = U$ and $K = U + P$ remain valid. However, the parameter δ becomes nonzero, due to the splitting between the two ground-state modes: $\sigma = 0$ and $\sigma = \Lambda$. This causes the dependence of the order parameters on μ/U to change as illustrated in figure 2. Note the difference between the order parameters for the two modes.

For the general case with $\theta \neq 0$, performing minimization over the axis rotations shows that the optimal squeezing occurs for the unrotated coordinate axes. By examining the spin squeezing parameter as a function of μ/U numerically, we find that particles are not entangled in the superfluid regime. We thus look for particle entanglement in the Mott phases.

With a small θ, the degeneracy in the ground states in the Mott phase is removed. In the $n = 1$ Mott phase, the ground state becomes $|g\rangle = |n_0 = 1, n_\lambda = 0\rangle$. For this state, the mean spin is along the direction of the axis-3 with $\langle T_3 \rangle = 1/2$ and $T_{1,2} = 0$. The spin fluctuations are given by $\langle \Delta T_{1,2}^2 \rangle = 1/4$ and $\langle \Delta T_3^2 \rangle = 0$. Employing a rotation by ϕ about the axis-3, we find that $\xi_{1',2'}^2 = 1$, i.e., the ground state is a CSS.

For the $n = 2$ Mott phase, we have a non-degenerate ground state of the form $|g\rangle = a|02\rangle + b|20\rangle$ [8] with
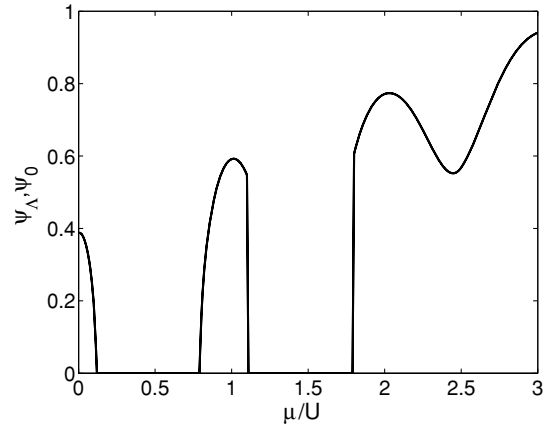
$$a = \left\{ \frac{1}{2} \left[1 - \frac{\Delta U - 2\delta}{\sqrt{(\Delta U - 2\delta)^2 + 4P^2}} \right] \right\}^{1/2}, \qquad (12)$$

$$b = \left\{ \frac{1}{2} \left[1 + \frac{\Delta U - 2\delta}{\sqrt{(\Delta U - 2\delta)^2 + 4P^2}} \right] \right\}^{1/2}. \qquad (13)$$

For such a state, as in the $n = 1$ Mott phase, the mean spin is pointed along the axis-3 with $\langle T_{1,2} \rangle = 0$ and $\langle T_3 \rangle = b^2 - a^2$. Their corresponding fluctuations are found to be $\langle \Delta T_1^2 \rangle = (a+b)^2/2$, $\langle \Delta T_2^2 \rangle = (a-b)^2/2$, and $\langle \Delta T_3^2 \rangle = 1 - (b^2 - a^2)^2$. To determine the optimum noise reduction and spin squeezing, we minimize over rotations about the mean spin (axis-3) direction by an angle ϕ. It is sufficient to consider either one of the rotated $1'$ or $2'$ axes so that a single rotation angle-dependent spin squeezing parameter ξ_ϕ^2 can be found as

$$\xi_\phi^2 = \frac{1 + 2ab\cos 2\phi}{(b^2 - a^2)^2}. \qquad (14)$$

Its minimum occurs at $\phi = \pm\pi/2$ such that $\xi_{\pm\pi/2}^2 = (1 - 2ab)/(b^2 - a^2)^2$. Assuming a small δ/P, we find $\xi_{\pm\pi/2}^2 \sim 1/2 + O((\delta/P)^2)$, in agreement with numerical calculation reported in figure 2. Thus, the ground state is particle entangled and spin squeezed.

We again calculate the concurrence values for the phases under consideration. It becomes zero everywhere except $n = 2$ Mott phase. In this situation $C(|g\rangle) = 2|ab|$ and for small δ/P values $C(|g\rangle) \sim 1 - O((\delta/P)^2)$. So that the results are in complete agreement with those of the squeezing parameter.

4.3. Antiferromagnetic regime

In this case, the atomic interaction parameter P is positive. In figure 3, the order parameters are plotted as a function of μ/U at $\theta = 0$.

Similar to the ferromagnetic regime, we first test the existence of spin squeezing for $\theta = 0$. The corresponding minimum squeezing parameter, ξ_2^2 for the fixed axes is shown
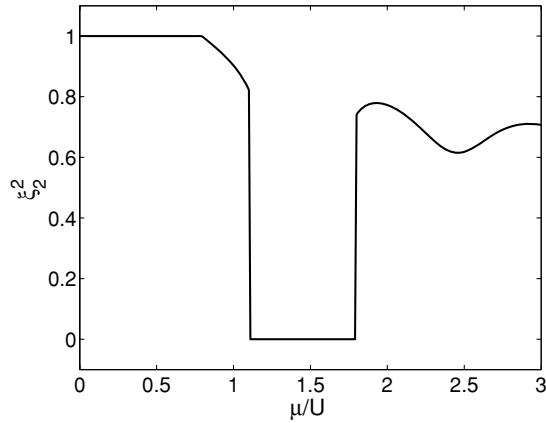
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Figure 4. The minimum squeezing parameter ξ_2^2 for the fixed axes configuration in the antiferromagnetic regime with $\theta = 0$, $J/U = 0.455 \times 10^{-1}$ and $P/U = 0.926 \times 10^{-2}$. $\xi_2^2 < 1$ denotes spin squeezing for the axis-2.

Figure 5. Concurrence versus μ/U in the antiferromagnetic regime with $\theta = 0$. The presence of pairwise entanglement is assured if the value of concurrence becomes larger than zero.

Figure 6. The order parameter ψ_0 for the antiferromagnetic regime at a small θ with $J/U = 0.455 \times 10^{-1}$, $P/U = 0.926 \times 10^{-2}$ and $\delta/U = 0.327 \times 10^{-2}$. $\psi_\Lambda = 0$ for these values of interaction parameters.

in figure 4. In contrast to the ferromagnetic case, squeezing is observed for the superfluid phase as well. In numerical calculations, we also rotate the coordinate system to see whether correlations can be enhanced for some angles. The optimum squeezing is found to occur for the fixed axes configurations.

In the $n = 1$ Mott phase, the ground state is a coherent superposition of $|10\rangle$ and $|01\rangle$, which identifies a manifold of any pure state for spin-1/2. The only difference is the quantization axis; it lies along the axis-2, instead of axis-1. Hence our conclusions for the ferromagnetic case remain applicable. The ground-state family is a general CSS and exhibits no squeezing, although mode entanglement can be present.

The $n = 2$ Mott-insulator state in the antiferromagnetic case, however, is significantly different from the ferromagnetic case considered earlier. It is no longer degenerate as before, and becomes uniquely determined as

$$|g\rangle = \tfrac{1}{\sqrt{2}}(|20\rangle + |02\rangle), \tag{15}$$

instead. For this special superposition state, the mean isospin vector becomes zero, with $\langle T_{1,2,3}\rangle = 0$. Spin fluctuations are found to be $\langle \Delta T_{1,3}^2\rangle = 1$ and $\langle \Delta T_2^2\rangle = 0$. Given in the second quantization form and in the occupation number representation, the mean number of particles in each mode $(0, \Lambda)$ is 1 and the state is mode entangled. In the first quantization, denoting single-particle wavefunctions as $\Psi_{i\sigma}$ for particles $i = 1, 2$ in modes $\sigma = 0, \Lambda$, $|g\rangle$ is found to become $|g\rangle = (1/\sqrt{2})(\Psi_{10}\Psi_{20} + \Psi_{1\Lambda}\Psi_{2\Lambda})$. This state has maximum quantum correlation among the particles and can be identified as a MES [31].

In order to compare the results measured in terms of the calculated concurrence, we show in figure 5 the dependence of concurrence as a function of μ/U.

The presence of particle entanglement in the superfluid phase is reflected by the nonzero values of concurrence for the corresponding μ/U values as shown in figure 5. Having a concurrence of one in the $n = 2$ Mott phase corresponds to the presence of a maximally entangled ground state.
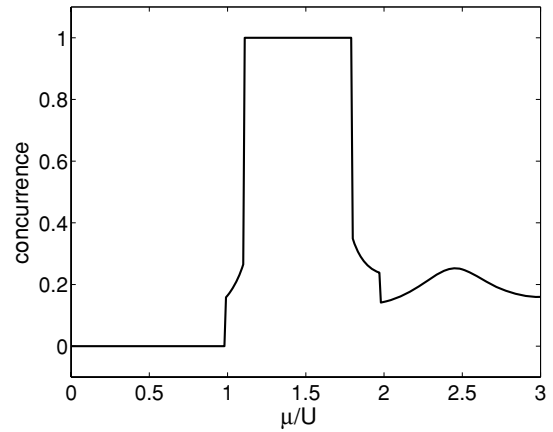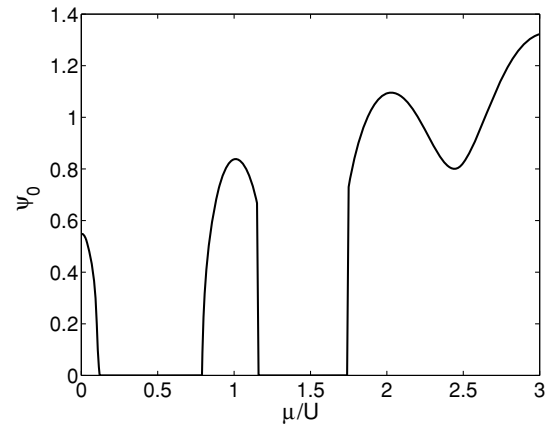
As was done previously for the ferromagnetic case, a small nonzero θ value can be introduced and the system parameters are changed accordingly. The corresponding graph for the order parameters as functions of μ/U are shown in figure 6.

Following the earlier procedure, the minimum squeezing parameter ξ_2^2 is also plotted against μ/U, with the optimized values, corresponding to the fixed coordinate system shown in figure 7.

As in the case of $\theta = 0$, spin squeezing is found to exist for the superfluid phase almost with the same strength. On the other hand, although spin squeezing is detected in the $n = 2$ Mott phase, it is reduced with a nonzero θ. The corresponding ground state for the $n = 2$ Mott phase is the same as in the ferromagnetic case. The MES of the $\theta = 0$ case for the antiferromagnetic interaction becomes a partially entangled state when a small nonzero θ is introduced.

The results from the calculated concurrence as shown in figure 8 are in complete agreement with those from the squeezing parameter. Squeezing is present in the superfluid phase and the maximal entanglement in the $n = 2$ Mott phase
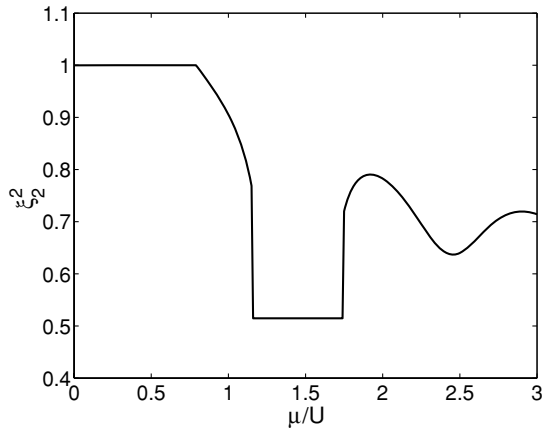
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Figure 7. The minimum squeezing parameter ξ_2^2 in the antiferromagnetic regime at a small θ in the fixed coordinate system with $J/U = 0.455 \times 10^{-1}$, $P/U = 0.926 \times 10^{-2}$ and $\delta/U = 0.327 \times 10^{-2}$.
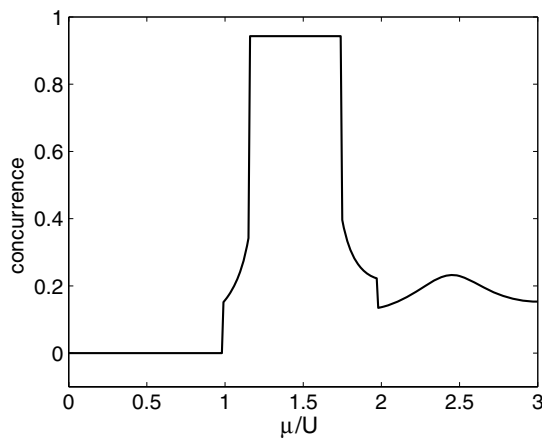

Figure 8. Concurrence at a small but nonzero θ in the antiferromagnetic regime. It is seen that part of the superfluid phase contains entangled particles.

becomes partially entangled with the introduction of a small but nonzero θ.

5. Conclusion

In summary, we have investigated quantum correlations between spin-1 bosons with coupled ground states in optical lattices. Both ferromagnetic and antiferromagnetic interactions are considered based on a model, initially developed in [8], that we believe can readily be adopted to current experimental systems. In addition to characterizing quantum correlations in various quantum phases in terms of coherent and squeezed spin states, and addressing both particle and mode entanglement, the role of lattice parameter in the familiar lin-θ-lin configuration is examined.

We have shown that for ferromagnetic interactions isospin squeezing (or multi-particle entanglement) is absent in the lattice model of spin-1 bosons in the superfluid phase. The one-particle Mott phase is in fact in a CSS, which is not particle

entangled, although it displays significant mode entanglement. The two-particle Mott state may contain SSS and entangled particles, if one of the degenerate components in the ground state manifold is made to dominant. It can be steered into a particle entangled state by introducing a nonzero θ to lift the degeneracy, while the CSS of the $n = 1$ Mott phase or the superfluid phase remains unentangled. The path to quantum entanglement is through the well-known single-axis twisting-type nonlinear interaction [19] for the degenerate ($\theta = 0$) case. With a nonzero θ, quantum entanglement is generated from a generalized LMG interaction, which includes a two-axis twisting type of spin–spin nonlinear interaction.

For antiferromagnetic interactions, spin squeezing and particle entanglement are found in both the $n = 2$ Mott and superfluid phases. In the $n = 2$ Mott state we find maximally entangled particles. Introducing a nonzero θ reduces this to a partially entangled state, and thus decreases particle correlations.

We compared the results of the squeezing parameter (7) with those of the concurrence (10) for each type of interaction and lattice configuration. They are in complete agreement in demonstrating the presence or absence of entanglement for the different phases.

For the system under consideration, we have investigated the potential ground states and the corresponding quantum correlations via examining entanglement/squeezing properties. Depending on the interaction parameters of the system, abrupt changes may occur if one considers the behaviour of entanglement properties. One can introduce symmetry-breaking perturbations to the Hamiltonian (5) to remove the degeneracy present in the various ground states. This can be done via including magnetic fields and Raman pulses with which adjustments to the ground-state populations in any particular spin components can be made [33]. As a specific example, generation of a coherent superposition of degenerate states (in this case Zeeman sublevels $M_F = \pm 1$) by stimulated Raman adiabatic passage scheme is demonstrated experimentally in [34].

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