Field-induced phase transitions of repulsive spin-1 bosons in optical lattices

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We study the phase diagram of repulsively interacting spin-1 bosons in optical lattices at unit filling, showing that an externally induced quadratic Zeeman effect may lead to a rich physics characterized by various phases and phase transitions. We find that the main properties of the system may be described by an effective field model, which provides the precise location of the phase boundaries for any dimension, being in excellent agreement with our numerical calculations for one-dimensional (1D) systems. Our work provides a quantitative guide for the experimental analysis of various types of field-induced quantum phase transitions in spin-1 lattice bosons. These transitions, which are precluded in spin-1/2 systems, may be realized using an externally modified quadratic Zeeman coupling, similar to recent experiments with spinor condensates in the continuum.

Ultracold atoms in optical lattices constitute a highly controllable scenario for the analysis of strongly-correlated systems, as highlighted by the realization of bosonic and fermionic Mott-insulators (MIs) [1,2]. Interestingly, on-going experiments [3,4] are approaching the regime at which magnetic properties, including the long-pursued Neél antiferromagnet in spin-1/2 fermions, could be revealed. Optically trapped spinor gases, formed by atoms with various Zeeman substates, are particularly interesting in this sense. The internal degrees of freedom result in an exceedingly rich physics, mostly by atoms with various Zeeman substates, are particularly interesting in this sense. The internal degrees of freedom result in an exceedingly rich physics, mostly characterized by various phases and phase transitions. We find that the main properties of the system may be described by an effective field model, which provides the precise location of the phase boundaries for any dimension, being in excellent agreement with our numerical calculations for one-dimensional (1D) systems. Our work provides a quantitative guide for the experimental analysis of various types of field-induced quantum phase transitions in spin-1 lattice bosons. These transitions, which are precluded in spin-1/2 systems, may be realized using an externally modified quadratic Zeeman coupling, similar to recent experiments with spinor condensates in the continuum.

Spin-1 gases are the simplest spinor system beyond the two-component one. Depending on interparticle interactions [6,7] (given by the s-wave scattering lengths $a_{s2}$ for collisions with total spin 0 and 2), spin-1 BECs present a ferromagnetic (FM) ground state (for $a_{s2} > a_0$ as in $^{87}$Rb $F = 1$ [8]) or an antiferromagnetic (AFM), also called polar, one (for $a_{s2} > a_0$, as in $^{23}$Na [8]). Spin-1 lattice bosons have also attracted a strong interest, especially the AFM case, for which a wealth of quantum phases have been predicted [9,10]. For AFM interactions, in 2D and 3D the MI states at odd filling are nematic [11,12,13], whereas in 1D quantum fluctuations lead to a spontaneously dimerized ground state [10,14,15,16,17,18]. The case $a_0 = a_2$ exhibits an enlarged $SU(3)$ symmetry with a highly degenerate ground state [19].

Most spin-1 species are naturally close to this $SU(3)$ point (i.e. $a_0 \approx a_2$), where external perturbations, as Zeeman shifts, may have a large effect, reducing the system symmetry, and thus favoring different phases. Since interactions preserve the magnetization, $M$, the linear Zeeman effect (LZE) may be effectively gauged out (although the phase diagram depends on $M$ [14,15]). On the contrary, the quadratic Zeeman effect (QZE) plays a crucial role in spinor gases. In spite of its importance, the role of the QZE in the quantum phases of spin-1 lattice bosons remains to a large extent unexplored, with the sole exception of the recent 3D mean-field analysis of Ref. [18], where it was shown that for finite $M$ the QZE may lead to nematic-to-ferromagnetic (or partially magnetic) transitions. This Letter discusses, for the first time to our knowledge, the complete phase diagram (Fig. 1) for MI phases (with unit filling) of spin-1 bosons in the presence of QZE, for the experimentally relevant case of a balanced mixture, i.e. with $M = 0$. Combining an effective field theory (for any dimension), 1D DMRG calculations, and exact Lanczos diagonalization, we obtain the phase boundaries, characterizing the phase transitions. We note that the QZE may be controlled by means of microwave and optical techniques [20,21]. Hence, as recently demonstrated for spinor BECs in the continuum [22], our results show that a controlled quenching of the QZE may permit the observation of field-induced phase transitions in spin-1 lattice bosons, which are precluded by simple

\begin{align*}
\theta &= \text{arctan}(J_2/J_1) - \pi \\
M &= \text{constant}
\end{align*}

FIG. 1: Mott phases of spin-1 lattice bosons at unit filling, as a function of $\theta \equiv \arctan(J_2/J_1) - \pi$ and the QZE $D$. Thick solid lines correspond to first order phase transitions for any $d$. Grey region is the dimerized phase (only in 1D). The symbols represent 1D numerical data (see text).
use of the LZE due to conservation of $\mathcal{M}$, and thus are absent in spin-1/2 systems. In addition, optical Feshbach resonances \[21, 28\] permit the modification of the ratio $a_2/a_0$, so that the full phase diagram discussed below may be explored with state of the art techniques.

We consider repulsively-interacting ultracold spin-1 bosons in a $d$-dimensional hypercubic lattice, prepared in a balanced mixture ($\mathcal{M} = 0$). The inter-particle interactions are characterized by the coupling constants $g_{0,2} = 4\pi\hbar^2 a_{0,2}/m_a$ (where $m_a$ is the atomic mass). At integer filling the system is in the MI regime if the (positive) interaction constants $g_{0,2} \gg t$, where $t$ is the hopping amplitude between neighboring sites. In second order of perturbation theory in $t$, the low-energy physics is given by super-exchange processes, being described by an effective bilinear-biquadratic spin Hamiltonian \[11, 13\]:

$$\hat{H}_I = -\sum_{\langle ij \rangle} \left[ J_1 \mathbf{S}_i \cdot \mathbf{S}_j + J_2 (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \right],$$

where $\mathbf{S}_i$ are spin-1 operators at lattice site $i$, the sum runs over nearest neighbors, $J_1 = 2t^2/g_2$ and $J_2 = 2t^2/3g_2 + 4t^2/3g_0$ (both are positive). Note that the FM case ($a_0 > a_2$) corresponds to $J_1 > J_2$, whereas the AFM case ($a_2 > a_0$) results in $J_2 > J_1$. As mentioned above, typically $a_0 \approx a_2$, which corresponds to the vicinity of the ferromagnetic $SU(3)$ point ($J_1 = J_2$).

As aforementioned, the QZE, characterized by the externally controllable constant $g$, plays a crucial role in the physics of the system. The QZE (which resembles the so-called single-ion term in other condensed-matter scenarios) leads to a modified Hamiltonian of the form

$$\hat{H} = \hat{H}_I - D J \sum_i (S_i^z)^2,$$

where $D = g/J$, with $J \equiv \sqrt{J_1^2 + J_2^2}$. In the following, we employ $J$ as the energy unit, setting $J = 1$, and introduce the standard parametrization of the exchange constants $J_1 = -J \cos(\theta)$, $J_2 = -J \sin(\theta)$, where the angle $\theta$ takes values in the interval $(-\pi, \pi)$ as the ratio $a_2/a_0$ varies from 0 to $\infty$ \[13\].

For $\theta < -3\pi/4 (J_1 > J_2)$ if $D \geq 0$ the ground state is a fully polarized ferromagnet in either $m = \pm 1$ (Ising-FM), and since $\mathcal{M} = 0$ phase separation into ferromagnetic $m = \pm 1$ domains is expected. For $D < 0$ the ground state for small values of $|D|$ is an XY-ferromagnet (XY-FM), i.e. the system fulfills $(S_i^z) = 0$, but presents a non-zero transversal magnetization. This phase is ordered in dimensions $d \geq 2$, exhibiting in 1D a quasi-long-range order with leading power-law decay of xy spin correlations. For larger $|D|$ (keeping $D < 0$) there is a phase transition between the XY-FM and the so-called large-$D$ phase (also called Ising-nematic), in which all atoms are in the $m = 0$ Zeeman substate, and hence all spin correlations decay exponentially. The field-induced phase transition between large-$D$ and XY-FM is discussed in detail below.

For $\theta > -3\pi/4 (J_1 < J_2)$ the dominant correlations are of spin-nematic (quadrupolar) type \[19, 21\]. A XY-nematic phase occurs for $D > 0$, characterized for $d \geq 2$ by $\langle (S^+)^2 \rangle \neq 0$ and $\langle \mathbf{S} \rangle = 0$, and in 1D by power-law correlations of the quadrupolar order parameter and exponentially decaying in-plane spin correlations. On the contrary, for $D < 0$ the large-$D$ phase is favoured. In 1D, for $D = 0$ a dimer nematic phase is expected \[10--14, 16, 21, 22\]. We show below that in 1D the QZE induces a transition between the dimer-nematic phase and the XY-nematic (or large-$D$) one.

To study the phase diagram near the $SU(3)$ point, we develop a low-energy effective field theory \[29\] based on spin-1 coherent states $|\psi\rangle = \sum_{a=x,y,z}(u_a + iv_a)|t_a\rangle$ where $|t_a\rangle$ are three Cartesian spin-1 states (Ising-FM is discussed in detail below. The average spin on a site fulfills $\mathbf{M} \equiv \langle \mathbf{S}|\mathbf{S}\rangle = 2(\mathbf{u} \cdot \mathbf{v})$

The FM region $\theta < -3\pi/4$ is characterized by $\mathbf{M}$ and the Euler angles ($\vartheta, \varphi, \chi$) which parametrize the orientation of the mutually orthogonal vector pair ($\mathbf{M}, \mathbf{u}$). The Euclidean Lagrangian for the model \[2\] takes then form:

$$L = i \sum_n \sum_{\langle \mathbf{M}_n \cdot \mathbf{M}_{n'} \rangle + J_2 \text{tr} (\mathbf{B}_n^T \cdot \mathbf{B}_n')},$$

where $B_{ab} = \langle \mathbf{S}|S^a S^b|\psi\rangle$ is related to the nematic tensor $Q = \frac{2}{3} \mathbf{B} - \mathbf{B}^T$ \[30\] and the magnetization $M_a = \epsilon_{abc} B_{bc}$. Assuming $\mathbf{u}$ and $\mathbf{v}$ as smooth fields, we may then pass to the continuum, performing a gradient expansion in Eq. \[3\]. For $D < 0$, configurations with $\vartheta \approx \pi/2$ and $\chi \approx 0$ are favoured. Since $(\vartheta, \varphi, \chi)$ is a pair of conjugate variables, $\vartheta$ and $\chi$ become “slaves” and can be integrated out (see Ref. \[29\] for details). The potential energy is minimized at $|\mathbf{M}| = M_0 = \{1 - \eta^2\}^{1/2}$, where $\eta = |D|/2Z(\sin \vartheta - \cos \theta)$, with $Z$ the lattice coordination number. We expand the effective action around the equilibrium value, $|\mathbf{M}| = M_0 + \delta$, integrate out $\delta$, and obtain the effective action for $\varphi$, which can be cast in the familiar form of the $(d + 1)$-dimensional XY model

$$A_{XY} = (\Lambda^{d-1}/2g) \int d^{d+1}x (\partial_\mu \varphi)^2.$$ 

Here $\Lambda$ is the ultraviolet lattice cutoff, and the coupling constant $g$, acting as an effective temperature, reads

$$g^2 = \frac{1}{2Z} \left\{ \frac{1 - \eta}{\eta} + \frac{\langle \delta^2 \rangle}{2\eta^2} \right\} \left\{ (1 - \eta) \right.$$

$$\times \left( \lambda + 1 + \eta \right) + \langle \delta^2 \rangle \left( 1 + \frac{\lambda}{2\eta} \right) \right\},$$

where $\langle \delta^2 \rangle = \langle \mathbf{S}|S^a S^b|\psi\rangle$. The fluctuation strength, $g_0^2 = (8Z\eta^2)/\langle \lambda + 2\eta^2 \rangle$ and $m_0^2 = \langle \delta^2 \rangle$.\[5\]
For a square lattice the resulting curve shown in Fig. 1, which, as mentioned above, agrees favorably with the known Monte-Carlo result for the classical 3D XY transition on a cubic lattice [33]. Extrapolating the peak position to the boundary is to study the fidelity susceptibility (FS) [32], where the quantity under the logarithm is the fidelity, obtained after adjusting the single fitting parameter \( g \). Once \( g \) is known, Eq. [5] constitutes an implicit equation to determine the transition curve \( D(\theta) \). The transition line has a universal slope for \( \lambda \to \infty \) (\( SU(3) \) point) given by \( \eta = 1 - O(\lambda^{-1/2}) \). Fig. 1 shows the curve for \( d = 1 \) obtained after adjusting the single fitting parameter \( g \) to the numerical results discussed below. An excellent agreement with the numerics is obtained for \( g \approx 0.6 \).

We have numerically evaluated the large-\( D \) to XY-FM boundary in 1D by means of DMRG calculations (following the method of Ref. [31] for up to 42 sites). We found that the most efficient way to locate the phase boundary is to study the fidelity susceptibility (FS) [32], which, as mentioned above, agrees favorably with the known Monte-Carlo result for the classical 3D XY transition on a cubic lattice [33]. Extrapolating the peak position to \( L = \infty \) yields the curve shown in Fig. 1 which, as mentioned above, agrees perfectly with the effective field-theoretical description after fitting the single parameter \( g \).

For \( d \geq 2 \), \( g \) may be estimated by neglecting fluctuations of \( M \) and demanding the critical \( |D| \) to match the Ising value \( Z J_1 \) at \( J_2 = 0 \), which yields \( g_e \approx (8Z/5\pi)^{1/2} \). For a square lattice the resulting \( g_e \approx 2.53 \) compares favorably with the known Monte-Carlo result \( g_e \approx 2.20 \) for the classical 3D XY transition on a cubic lattice [33]. The corresponding transition curves obtained from the implicit Eq. [5] are also shown in Fig. 1.

For the AFM region, \( \theta > -3\pi/4 \), the effective theory can be formulated in terms of the nematic director \( \mathbf{u} \) [29], or alternatively via the nematic tensor \( Q^{ab} = u_a u_b - \delta_{ab}/3 \)

\[
A_n = (\Lambda^d - 1/4g_n) \int d^{d+1} x \{ (\partial_{\mu} Q^{ab})^2 + 2\Lambda^2 m_n^2 Q^{zz} \} \tag{6}
\]

where the coupling \( g_n = \sqrt{Z/2\Lambda} \) vanishes at the \( SU(3) \) point [29] and \( m_n^2 = D/\sin \theta \) is the QZE-induced mass. The \( \mathbf{u} \) anisotropy is of the easy-plane (easy-axis) type for \( D > 0 \) (\( D < 0 \)). For \( d \geq 2 \) there is a long range nematic order for any \( D \), with a single transition at \( D = 0 \), between a gapless XY-nematic phase with \( \langle S^z \rangle^2 \neq 0 \) at \( D > 0 \) and a gapped Ising-nematic \( \langle S^z \rangle^2 \) = 0 at \( D < 0 \).

For \( d = 1 \), at \( D = 0 \) the AFM phase presents exponentially decaying nematic correlations (albeit with a very large correlation length \( \xi \approx e^{2\pi/g_n} \)) and a tiny spin gap \( D \approx \xi^{-1} \) close to the \( SU(3) \) point [20, 21]. In this phase the lowest excitations have total spin \( S = 2 \), which can be understood by noticing that in model (4) the magnetization \( M \) is a composite field, \( M = \exp\{Q^{bd} (\theta - Q^{cd}) \} \). \( Q^{ab} \) can be approximated as a free field with finite mass \( m = D^{1/2} \), so its correlator corresponding to \( S = 2 \) excitations decays as \( e^{-2\pi/g_n} \), while the spin correlator describing \( S = 1 \) excitations decays much faster, as \( e^{-2\pi/g_n} \). However, as aforementioned, this featureless disordered-nematic phase [20, 21] acquires a very weak long-range dimer order all the way to the \( SU(3) \) point, due to the condensation of \( Z_2 \) disclinations [12, 34]. Although model (4) cannot describe dimerization, it may be employed to determine the boundaries of XY-Nematic and Ising nematic phases at very small \( |D| \), provided that \( Z_2 \) disclinations do not play role at the corresponding phase transitions. When \( D > 0 \), this transition is KT, and the transition line close to the \( SU(3) \) point fulfills \( D = C J_2 \exp\{-4\pi(1 - J_1/J_2)^{-1/2} \} \), where \( C > 0 \) is a numerical constant. At \( D < 0 \) the phase transition is Ising-like, with a boundary similar as for \( D > 0 \), but a negative constant \( C \). As shown below, this analysis provides a good insight on the dimer-to-nematic transitions.

To characterize numerically the boundaries of the dimerized phase (where FS remains featureless), we employed level spectroscopy analysis [35]. In a finite chain, two dimerized ground states (degenerate in the thermodynamic limit) split in energy, so the lowest excited state in the dimerized phase is unique and belongs to the \( M = 0 \) sector. In contrast, both in the large-\( D \) phase (\( D < D_c^- \)) and in the XY-nematic (\( D > D_c^+ \)), the lowest excited states are twofold degenerate, having \( M = \pm 1 \) and \( M = \pm 2 \), respectively. Thus, in finite chains a level crossing between the lowest excited singlet and doublet states occurs when changing \( D \). Our extrapolated results for \( D_c^+ \), obtained by Lanczos diagonalization for periodic systems of up to \( L = 16 \) sites, are shown in Fig. 1 with \( \Delta \to D_c^-, \square \to D_c^- \). Note that
when approaching the $SU(3)$ point our numerics cannot recover the exponentially small dimer region, which basically reduces to $D = 0$ line. The finite size extrapolation of $D^+$ follows $1/L^2$ law, confirming its KT nature.

To determine the universality class of the $D = D^-$ transition, we have computed the central charge at $D = 0$, $\theta = -0.73\pi$. The block entanglement entropy for an open 1D system of size $L$, divided into two pieces of size $l$ (block) and $L-l$ (environment), behaves as $S = \frac{1}{4} \log \left( \frac{1}{2} \sin \left( \frac{\pi l}{L} \right) \right) + A$, where $c$ is the central charge and $A$ is a non-universal constant. Setting $l = \frac{L}{2}$, following Ref. [39], and using DMRG to evaluate $S$ for several $L$ values, we obtain $c \approx 1.5$. The $D = D^-$ KT line has $c = 1$; subtracting its contribution, we get $c = \frac{3}{2}$ for the $D = D^-$ line, confirming its Ising nature.

Finally, we discuss the behavior of the chirality $\tau = \frac{1}{2} \sum_i \langle \hat{n}_{i+1} \hat{n}_{i-1} - 2 \hat{n}_{i} \rangle$, which can be easily monitored in Stern-Gerlach-like time-of-flight experiments. Figure 2(b) shows $\tau$ as a function of $D$. At the FM side, $\tau$ is discontinuous at $D = 0$ indicating the first-order character of the transition, which is clear since for the Ising-FM phase ($D > 0$) $\tau = 1$, while in the XY-FM phase ($D < 0$) for $D \to 0$ the ground state energy is minimized at $(M, \vartheta, \chi) = (1, \frac{\pi}{2}, 0)$, and thus for $\langle \hat{S}_x^2 \rangle \to \frac{1}{2}$ and $\tau \to -\frac{1}{2}$. At the XY-FM to large-D transition, $\tau$ practically saturates to $-\frac{1}{2}$ for a value of $D$ close to that obtained from the FS analysis. On the AFM side the limit $D \to 0$ is non-singular and thus $\tau = 0$ there. The nematic-to-dimer transitions do not present any pronounced feature of $\tau$. These transitions could be revealed experimentally by Faraday rotation techniques [10] or those recently explored in Ref. [11].

In summary, we have obtained the complete phase diagram (for any dimension) for spin-1 lattice bosons in the MI phase (at unit filling) in the presence of quadratic Zeeman coupling. Our results provide hence a quantitative guide for the analysis of field-induced quantum phase transitions in lattice bosons, which, similar to recent experiments with spinor BECs in the continuum [24], may be realized modifying the QZE by means of microwave dressing. Starting in the large-D phase, and dynamically modifying the QZE across the transitions discussed in this paper, should result in the FM regime in the appearance of XY-FM domains, similar to those observed in spin-1 BECs [24], whereas quenches in the AFM regime should lead to nematic domains with different $\langle \hat{S}_{x,y}^2 \rangle$ but homogeneous $\langle \hat{S} \rangle = 0$. We stress that such field-induced transitions are precluded for spin-1/2, constituting an interesting novel feature of lattice spinor gases.

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