Magnetization Plateaus for Spin-One Bosons in Optical Lattices: Stern-Gerlach Experiments with Strongly Correlated Atoms

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We consider insulating states of spin-one bosons in optical lattices in the presence of a weak magnetic field. For the states with more than one atom per lattice site we find a series of quantum phase transitions between states with fixed magnetization and a canted nematic phase. In the presence of a global confining potential, this unusual phase diagram leads to several novel phenomena, including the formation of magnetization plateaus. We discuss how these effects can be observed using spatially resolved spin polarization measurements.

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Far-off-resonance optical traps can confine neutral atoms regardless of their hyperfine state [1] and open exciting possibilities for exploring multicomponent systems of degenerate atoms [2–16]. Experimental studies of the hyperfine spin-one manifold of ^{23}Na atoms confined in a single optical trap already revealed the ground state spin structure in an external magnetic field [17], the formation and persistence of the metastable spin domain configurations [18], and quantum tunneling across spin domain boundaries [19]. These phenomena have been understood using mean-field theory [2,3,20] since in a large trap, atoms can be considered as weakly interacting. At the same time, theoretically predicted many-body features of spin-one condensates, such as a spin singlet nature of the ground state for an even number of atoms [4], could not be observed in such experiments since the energy difference between various spin states is inversely proportional to the volume of the system and is extremely small for realistic traps [5,6].

Several approaches have been suggested for creating strongly correlated quantum states of spinor atoms in optical lattices produced by standing wave laser fields [7–11]. In the presence of a deep optical lattice, wave functions of atoms are localized near the lattice potential minima, which leads to a strong enhancement of interactions between atoms [21–23] and can result in dramatic changes in the properties of ultracold gases. It is also important that in optical lattices one can have a small number of atoms per lattice site (in experiments of Ref. [22], this number was around 1–3). In an insulating state, hopping between different sites is negligible and each well behaves essentially as a small condensate. In this regime, the behavior of spin-one bosons in each well will be dominated by the strong spin-spin interactions such as those predicted by [4]. Two component atom mixtures in optical lattices have already been realized in experiments of Ref. [24].

Nontrivial nature of the ground state of localized spin-one bosons in optical lattices has been discussed previously in [7–9]. Virtual hoppings of the atoms give rise to spin exchange interactions between neighboring sites and lead to several distinct insulating phases that differ in their spin correlations. In two and three-dimensional lattices, states with odd numbers of particles per site are always nematic, and for states with even numbers of particles per site, there is always a spin singlet phase, and there may also be a first order transition into the nematic phase. In this Letter we extend earlier analysis and show that in a magnetic field, insulating states with more than one atom per site undergo a series of phase transitions between spin gapped phases with quantized magnetization and phases with so-called canted nematic order in which magnetization can vary continuously. The critical properties of these phase transitions have been recently investigated in [25]. A magnetic phase diagram is similar to the phase diagram of the spinless boson Hubbard model: states with quantized magnetization are analogous to the Mott insulating phases, while the canted nematic phase is analogous to the superfluid phase. We also propose two kinds of experiments that can verify the presence of such magnetization plateaus and demonstrate the many-body nature of insulating states of spin-one bosons in optical lattices.

An effective Hamiltonian for spin-one bosons in an optical lattice in the presence of a magnetic field is given by [8]

$$\mathcal{H} = -t\sum_{\langle ij\rangle,\sigma}(a_{i\sigma}^\dagger a_{j\sigma} + a_{j\sigma}^\dagger a_{i\sigma}) + \frac{U_0}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + \frac{U_2}{2}\sum_i(\vec{S}_i^2 - 2\hat{n}_i) - \mu\sum_i \hat{n}_i - H\sum_i S_{zi}. \quad (1)$$

Here, $a_{i\sigma}^\dagger$ are creation operators for particles in the lowest Bloch band localized on site i and having spin components $\sigma = 0, \pm 1$; $n_i = \sum_\sigma a_{i\sigma}^\dagger a_{i\sigma}$ and $\vec{S}_i = \sum_{\sigma\sigma'} a_{i\sigma}^\dagger \vec{T}_{\sigma\sigma'} a_{i\sigma'}$ are the number and spin operators for site i ($\vec{T}_{\sigma\sigma'}$ are the usual spin matrices for spin one particles). For each well, the collective spin of the atoms

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satisfies constraints $S_i \leq N_i$, and $S_i + N_i$ is even. Parameters t, U_0 and U_2 for a realistic case of a three-dimensional cubic lattice have been obtained in [8]. The ratio of the interaction terms in (1), U_2/U_0, is fixed by the ratio of the scattering lengths and is independent of the nature of the lattice. Scattering lengths of ^{23}Na obtained in Ref. [26] give $U_2/U_0 = 0.04$. In this Letter we neglect effects of the quadratic Zeeman shift since magnetization plateaus that we are interested in appear for magnetic fields of the order of mGauss (assuming a typical $U_2 \approx 0.1$ kHz).

When the spin dependent interaction (U_2) is much smaller than the Hubbard repulsion (U_0), the superfluid-insulator transition [23,27] is determined mostly by U_0. The spin gap U_2 term, however, is important inside the insulating regime, in which nontrivial spin phases appear as a result of a competition between a spin gap, a magnetic field, and spin exchange interactions, induced by fluctuations in the particle number. The magnetic phase diagram can be most easily understood by considering the limit of large number of atoms per site, $N \gg 1$. In this case the effective spin Hamiltonian for the insulating state can be written as a model of quantum rotors, interacting via rotationally invariant quadrupolar interaction [8,9]:

$$\mathcal{H} = \sum_i \frac{U_2}{2} \vec{S}_i^2 - H S_{zi} - \frac{2N^2 t^2}{U_0} \sum_{ij} n_{ia} n_{ib} n_{ja} n_{jb}. \quad (2)$$

Angular momentum $\vec{S}_i = -i\mathbf{n}_i \times \frac{\partial}{\partial \mathbf{n}_i}$ describes the collective spin on site i and inherits constraints of the microscopic Hamiltonian (1). In the mean-field approximation [28,29] we replace (2) by a sum of single site Hamiltonians

$$H_{MF,i} = \frac{U_2}{2} \vec{S}_i^2 - H S_{zi} - \frac{zN^2 t^2}{U_0} \left(Q_{ab} + \frac{1}{3} \delta_{ab} \right) n_{ia} n_{ib}, \quad (3)$$

with z being the number of nearest neighbors, and impose a self-consistency condition on the nematic order parameter $Q_{ab} = \langle n_{ia} n_{ib} \rangle - \frac{1}{3} \delta_{ab}$. Magnetic phase diagrams obtained by solving (3) self-consistently for the cases of odd and even filling factors are shown in Figs. 1 and 2 (for details, see [30]). When $t = 0$ the Hamiltonian (3) does not mix different spin eigenstates. In a magnetic field, the system has a series of level crossings between states with different values of the spin. Each of these states has a gap in the excitation spectrum and remains stable after turning on a finite value of t. This results in lobes of fixed magnetization shown in Figs. 1 and 2. Only at points where spin eigenstates come into degeneracy do exchange interactions give rise to mixing of different spin eigenstates, leading to a Canted Nematic phase. The latter has an expectation value of the nematic order parameter Q_{ab} in a plane perpendicular to the magnetic field [25]. Hence, it has spontaneous breaking of the symmetry of spin rotations around the direction of magnetic field. For sufficiently large magnetic field the system becomes fully polarized with $S_i = N$. We note that for $N = 1$ and $N = 2$ one can derive effective spin interactions that do not rely on the large N approximation of Eq. (2) [8]. These models give magnetic phase diagrams that are qualitatively similar to Figs. 1 and 2 [30]. We also point out that inside the lobes of fixed magnetization and in the mean-field approximation the many-body wave functions factorize $|\Psi\rangle = \prod_i |S_i = S, S_{iz} = S\rangle$.

A typical experimental system has a parabolic confining potential in addition to the periodic optical lattice. This means that the chemical potential is not uniform, and for small t, the system breaks into insulating domains with different integer filling factors, separated by regions of the superfluid phase (see Refs. [23,31] for analysis of the spinless case). Another important experimental constraint is that the total magnetization is fixed by the initial state of the system. In the discussion above, we showed that when we change magnetic field, it is energetically favorable to adjust the magnetization in order to utilize some of the Zeeman energy (see Figs. 1 and 2). From Eq. (1) we observe, however, that the spin component parallel to the applied field is conserved. For example, if the magnetic field is along the z-axis, $S_{\text{tot,z}} = \sum_i S_{iz}$ is a good quantum number of the system (spin nonconserving interactions, such as the dipolar relaxation, are typically small) and should not change even when H_z is changing. For a single large trap, this feature allowed to study magnetic properties of spinor condensate [17] at magnetic

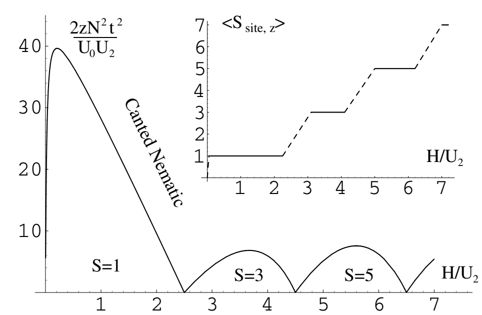

FIG. 1. Magnetic insulating phase of spin-one bosons in optical lattice with an *odd* number of atoms per site N. Magnetization is fixed inside the lobes but varies continuously inside the Canted Nematic phase. The latter has an expectation value of the nematic order parameter Q_{ab} in the plane perpendicular to the direction of magnetic field. For sufficiently large magnetic field the system becomes fully polarized with $S = N$ (not shown here). The insert shows the ground state magnetization (per site) as a function of magnetic field for $2zN^2t^2/U_0 = 5U_2$. Note that near $H = 0$, magnetization grows linearly with magnetic field and quickly reaches the $S_{\text{site,z}} = 1$ plateau.

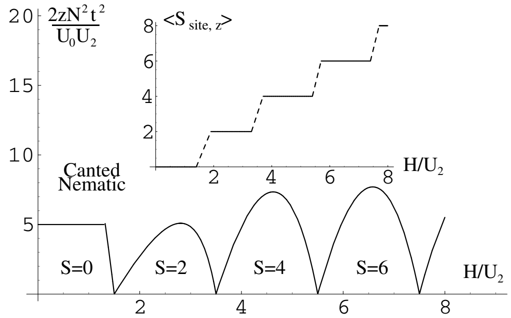

FIG. 2. Magnetic insulating phase in optical lattice with an *even* number of atoms per site. The insert is for $2zN^2t^2/U_0 = 2U_2$.

fields for which the true ground state should be fully polarized.

A way around spin conservation has been demonstrated in [17] and relies on applying spatially varying magnetic fields and performing Stern-Gerlach imaging. Here we extend these ideas and suggest an approach to experimental observation of the magnetization plateaus discussed above. The idea of our first experiment is shown in Fig. 3. We consider a strongly anisotropic trap in which a magnetic field gradient is applied parallel to the long axis of the system. When there is a magnetic field gradient parallel to the long axis, there should also be gradients in the transverse directions (both $\vec{\nabla}\vec{H}$ and $\vec{\nabla}\times\vec{H}$ should be zero). We assume that the size of the condensate in the transverse directions is small enough that we can neglect the effects of the magnetic field in transverse directions. However, the size of the condensate should be larger than the optical lattice period in any direction, so that we can consider it as a three-dimensional system. As we discussed before, the uniform part of the magnetic field has no effect on the state of the system, so in our discussion we set it to zero. To be concrete, we assume that the largest insulating domain at the center of the trap has a filling factor $N = 6$ and that our system has been prepared to have $S_{\mathrm{tot,z}} = 0$. In a nonuniform magnetic field, different parts of the $N = 6$ domain minimize their energy for different values of magnetization. When the field gradient is sufficiently large and tunneling is small enough, the locally favored magnetization changes in a steplike fashion from $S_{\mathrm{site,z}} = -6$ (per site) on the left to $S_{\mathrm{site,z}} = 6$ on the right. Such state is also consistent with the spin conservation, since $S_{\mathrm{tot,z}}$ remains zero. So, the configuration that minimizes the energy has plateaus in the spatial profile of magnetization, with spin polarizations (per atom) $S_{\mathrm{atom,z}} = -1, -2/3, -1/3, 0, 1/3, 2/3, 1$, as shown in Fig. 3. Each plateau has a length of the order of $2U_2/|\nabla H|$. The appearance of spin plateaus in a nonuniform magnetic field is analogous to the domain structure of condensates in optical lattices in the presence of a nonuniform global confining potential that was discussed before [23,31]. In the latter case, the total density is fixed by the number of atoms in the trap, but insulating phases with different integer filling factors exist due to the confining potential. To detect the magnetization plateaus shown in Fig. 3, one needs to image different parts of the trap separately, measuring spin polarization per atom as a function of the position: $\langle S_{\mathrm{atom,z}}\rangle = (n_+ - n_-)/(n_+ + n_0 + n_-)$, where $n_\pm$, n_0 are the local densities of atoms with $\sigma = \pm 1$ and 0, respectively. This quantity can be most easily measured in Stern-Gerlach time-of-flight experiments. If a small gradient of magnetic field is applied during expansion, clouds with different spin components spatially separate, and one can measure the number of atoms with different spin components using light scattering.

To illustrate system parameters needed to realize this experiment we consider a cigar shaped condensate of sizes $400 \times 10 \times 10$ μm. For an optical lattice created with $\lambda = 985$ nm lasers and 4×10^5 atoms in a condensate, we get the maximum density of six atoms per well in the center of the trap. To observe five plateaus in this setup, one would need magnetic field gradients $\sim$100 mG/cm and a spatial resolution of 30 μm. These parameters have already been achieved in experiments of Ref. [17]. Inside the insulating phase the characteristic time scale for spin relaxation between different wells is set by the exchange interactions $\tau_{ex} = \hbar U_0/(Nt)^2$. For $t = 0.1$ khz and $U_0 = 2$ khz we find times of the order of hundreds of milliseconds. So, if a magnetic field gradient is applied in the insulating regime, one needs to wait at least that long for magnetic plateaus to develop. Experimentally it may be more efficient to apply magnetic field gradient when the system is in the superfluid regime and then take the system to the insulating state by slowly reducing t.

We now discuss our second "spin decoration" approach to experimental detection of spin gap effects in the insulating regime of spin-one bosons. The idea of this method is that when a system is prepared with a nonzero

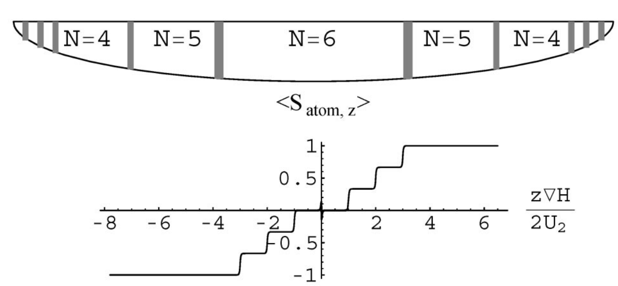

FIG. 3. A system of spin-one bosons in an optical lattice confined by a parabolic potential. In the insulating regime the cloud breaks into insulating domains with different integer filling factors. When magnetic field gradient is applied parallel to the long axis of the trap, magnetization plateaus develop inside individual insulating domains.

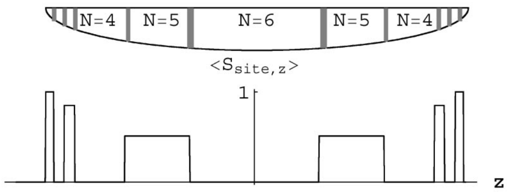

FIG. 4. A system of spin-one bosons with a nonzero total magnetization in an optical lattice (no external magnetic field). Magnetization gets distributed among regions with odd filling factors and is pushed out of the regions with even fillings.

magnetization in the absence of magnetic field gradients, magnetization gets distributed nonuniformly among insulating domains with different filling factors. Spin polarization appears predominantly in domains with odd numbers of atoms per site and is pushed out of the regions with even fillings. To justify this conjecture we propose the following argument. In the regime, when tunneling is small ($zN^2t^2/U_0 \ll U_2$), there is a crucial difference in spin susceptibility between odd and even phases. For even domains, one needs to pay an energy $3U_2$ to break a singlet state and have $S_{\mathrm{site,z}} \sim 2$. For odd sites the lowest energy state already has $S = 1$, and energy cost to polarize existing spins is of the order of zN^2t^2/U_0. Therefore, externally imposed nonzero magnetization will be redistributed in odd insulating domains. For small magnetization per site, energy goes as

$$E_{\mathrm{odd}}(N, S_{\mathrm{site,z}}) = \frac{1}{2\chi_{\mathrm{odd}}(N)} S^2_{\mathrm{site,z}}, \tag{4}$$

where $\chi_{\mathrm{odd}}(N)$ is a spin susceptibility of the sites with odd filling factor N. If $\chi_{\mathrm{odd}}(N)$ was the same for all N, then magnetization would be distributed uniformly among all odd domains. In reality, $\chi_{\mathrm{odd}}(N)$ decreases with increasing N, so we expect larger magnetization for insulating domains with smaller numbers of atoms. Quadratic dependence in (4) ensures, however, that all domains with odd filing factors acquire finite magnetization. So, in experiments we expect to find a picture of alternating even and odd domains, in which odd domains have finite magnetization and even domains have none (see Fig. 4). This picture is valid until all odd regions have magnetization $S_{\mathrm{site,z}} = 1$. For the experimental setup discussed earlier, this corresponds to $\langle S_{\mathrm{atom},z}\rangle \lesssim 0.1$. By performing spatially resolved measurements of spin polarization, one should be able to observe such a modulated structure of magnetization.

In summary, we discussed insulating states of spin-one bosons in optical lattices in the presence of a magnetic field. For systems with more than one particle per site we demonstrated the existence of a series of phase transitions between phases with fixed magnetization and the canted nematic phase in which magnetization can vary continuously. We considered experimental signatures of this novel magnetic phase diagram, including formation of magnetization plateaus in the presence of a magnetic field gradient and a modulated spin density in nonuniform systems with nonzero total magnetization.

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