First-order superfluid to Mott-insulator phase transitions in spinor condensates

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We observe evidence of first-order superfluid to Mott-insulator quantum phase transitions in a lattice-confined antiferromagnetic spinor Bose-Einstein condensate. The observed signatures include hysteresis effect and significant heatings across the phase transitions. The nature of the phase transitions is found to strongly depend on the ratio of the quadratic Zeeman energy to the spin-dependent interaction. Our observations are qualitatively understood by the mean field theory, and in addition suggest tuning the quadratic Zeeman energy is a new approach to realize superfluid to Mott-insulator phase transitions.

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A quantum phase transition from a superfluid (SF) to a Mott-insulator (MI) was realized in a scalar Bose-Einstein condensate (BEC) trapped by three-dimensional (3D) optical lattices around a decade ago [1]. Marking an important milestone, this achievement has stimulated tremendous efforts to apply highly controllable ultracold bosonic and fermionic systems in studying condensed matter models [2–6]. The SF-MI transitions have been confirmed in various scalar BEC systems via different techniques that can efficiently control the ratio of interatomic interactions to the mobility of atoms [1, 5–7]. One well-known approach to simultaneously enhance interatomic interactions and suppress atomic motion is by raising the depth of an optical lattice [8]. Another convenient method is to manipulate interactions with a magnetically tuned Feshbach resonance [9]. A third technique is to control the hopping energy of bosonic atoms by periodically shaking the lattice [10]. Spinor BECs, on the other hand, possess an additional spin degree of freedom, leading to a range of phenomena absent in scalar BECs [8–13]. One important prediction is the existence of the first-order SF-MI phase transitions in lattice-trapped antiferromagnetic spinor BECs [2, 14–17]. In contrast, the phase transitions can only be second order in scalar BECs and ferromagnetic spinor BECs [12, 18, 19].

In this paper, SF-MI phase transitions are studied in sodium antiferromagnetic spinor BECs confined by cubic optical lattices. We observe hysteresis effect and substantial heating across the phase transitions, which indicate the existence of meta-stable states and associated first-order transitions. In the ground state of the spinor BECs, the nature of the SF-MI transitions is found to be determined by the competition between the quadratic Zeeman energy $q_B$ and the spin-dependent interaction $U_2$. At low magnetic fields where $U_2$ dominates, signatures of first-order transitions are observed. In the opposite limit, the transitions appear to be second order and resemble those occurring in scalar BECs. These qualitative features are explained by our mean-field (MF) calculations. We also study the phase transitions with an initial meta-stable state and observe stronger heating across all magnetic fields. Furthermore, our data indicate that a new technique to realize SF-MI transitions is by varying $q_B$.

Similar to Refs [12, 18], we describe a lattice-trapped $F = 1$ spinor BEC with the Bose-Hubbard model in the lowest band as follows,

$$H = \frac{U_0}{2} \sum_i n_i (n_i - 1) - J \sum_{\langle i,j \rangle, m_F} b_{i,m_F}^\dagger b_{j,m_F} - \mu \sum_i n_i + \frac{U_2}{2} \sum_i (\langle \hat{S}_i^2 \rangle - 2n_i) + q_B \sum_{i,m_F} m_F^2 n_{i,m_F}. \quad (1)$$

Here $J$ is the nearest-neighbor hopping energy, $n_i = \sum_{m_F} n_{i,m_F}$, and $n_{i,m_F} = b_{i,m_F}^\dagger b_{i,m_F}$ is the atom number of the $m_F$ hyperfine state at site $i$. $U_0$ characterizes the spin-independent interaction, $\mu$ is the chemical potential, and $\hat{S}_i$ is the spin operator at site $i$. $U_2$ is positive (negative) in an antiferromagnetic (ferromagnetic) spinor BECs, e.g., $U_2 \simeq 0.04U_0$ in our $^{23}\text{Na}$ system [20]. By neglecting the second order term $(b_{i,m_F}^\dagger - b_{i,m_F})(b_{j,m_F} - b_{j,m_F}^\dagger)$ in the hoppings and applying the decoupling MF theory, Eq. (1) can be reduced to a site-independent form [12, 21, 22],

$$H_{MF} = \frac{U_0}{2} n(n-1) + \frac{U_2}{2} \langle \hat{S}_i^2 \rangle - 2n + q_B \sum_{m_F} m_F^2 n_{m_F} - zJ \sum_{m_F} (\phi_{m_F}^\dagger b_{m_F} + \phi_{m_F} b_{m_F}^\dagger) + zJ|\phi|^2 - \mu n \quad (2)$$

with the vector order parameter being $\phi_{m_F} \equiv \langle b_{m_F} \rangle$ and $z$ being the number of nearest neighbors. With spatially uniform superfluids in equilibrium, one can assume $\phi_{m_F} = 0 \ (\neq 0)$ in the MI (SF) phase.

An antiferromagnetic $F = 1$ spinor BEC of zero magnetization forms a polar superfluid in equilibrium with $\langle \hat{S}_i \rangle = 0$ [23, 24]. There are two types of polar superfluids: the longitudinal polar (LP) state with $(\phi_1, \phi_0, \phi_{-1}) = \sqrt{2} \phi_0(0,1,0)$ and the transverse polar
For LP and TP at $q_b = 0$: MI, MSF, MMI. MI for LP at $q_b/h = 400$ Hz. MI for scalar.

Other regions are SF.

 FIG. 1. (Color online) (a) MF phase diagrams derived from the Bose-Hubbard model for scalar BECs [18], and the LP and TP sodium spinor BECs in cubic lattices (see Eq. (2)). The SF order parameter versus $u_L$ in (b) scalar and (c) LP/TP spinor BECs at $\mu/U_0 = 1.4$, i.e., along the dotted line in Panel(a). Note that SF-MI transitions are second order in a scalar BEC, and they are first order showing hysteresis effect in LP and TP spinor BECs at $\mu/U_0 = 1.4$ and $q_b = 0$. (d) Predicted SF-MI transition point $u_c$ versus $q_b$ after cubic lattices are ramped up and down at $\mu/U_0 = 1.4$ (see Eq. (2)).

\[ (TP) \text{ state with } \langle \phi_1, \phi_0, \phi_{-1} \rangle = \sqrt{\rho_s/2}(1, 0, 1), \text{ where } \rho_s \text{ is the number of condensed atoms per site. At } q_b = 0, \text{ TP and LP states are degenerate in energy when they have the same } \rho_s. \text{ At } q_b > 0, \text{ the MF ground state is always the LP state, although a meta-stable TP phase may also exist} [3, 24]. \text{ We solve Eq. (2) self-consistently by requiring } \phi_{m_F} = \langle \phi_{m_F} \rangle \text{ in the occupancy number basis with a maximum of 15 atoms per site. Since the observed peak occupancy number is around six, the truncation errors are negligible.}

Our MF calculations show that $q_B/U_2$ is a key factor to understand the nature of SF-MI transitions in antiferromagnetic spinor BECs. At low magnetic fields (where $0 \leq q_B \lesssim U_2$), $U_2$ penalizes high-spin configurations and enlarges the Mott lobes for even number fillings as atoms can form spin singlets to minimize the energy. Meta-stable Mott-insulator (MMI) and meta-stable superfluid (MSF) phases emerge due to the spin barrier, and lead to first-order SF-MI phase transitions (see Figs. 1(a) and 1(c)) [14, 10, 17]. When 3D lattices are ramped up and down, hysteresis is expected across the phase transitions (i.e., different transition lattice depth $u_c$). In addition, when the system changes from a meta-stable phase to a stable phase (e.g., from a MSF phase to a MI phase), there will be a jump in the order parameter and the system energy, leading to unavoidable heating to the atoms. Hence, hysteresis and substantial heating may be interpreted as signatures of first-order transitions. As $q_B$ increases, the $m_F = 0$ state has lower energy than other $m_F$ levels and $U_2$ becomes less relevant. When $q_B$ becomes sufficiently larger than $U_2$ ($U_2/h \lesssim 80$ Hz in this work), the ground state phase diagram of antiferromagnetic spinor BECs reverts back to one that is similar to the scalar Bose-Hubbard model with only second-order SF-MI transitions (see Figs. 1(a), 1(b) and 1(d)).

Three different types of BECs (i.e., scalar BECs, LP and TP spinor BECs) are studied in this work. A scalar BEC containing up to $1.2 \times 10^5$ sodium atoms in the $|F = 1, m_F = -1 \rangle$ state is created with an all-optical approach (see Ref. 26). A $F = 1$ spinor BEC of zero magnetization is then produced by imposing a resonant rf-pulse to the scalar BEC at a fixed $q_B$. Since the LP state is the MF ground state, it can be prepared by simply holding the spinor BEC for a sufficiently long time at high magnetic fields [24]. A different approach is required to generate the TP state: we apply a resonant microwave pulse to transfer all $m_F = 0$ atoms in the $F = 1$ spinor BEC to the $F = 2$ state, and then blast away these $F = 2$ atoms with a resonant laser pulse. After quenching $q_B$ to a desired value, we adiabatically load the BEC into a cubic lattice by linearly raising the lattice depth $u_L$.

FIG. 2. (Color online) (a) Schematic of the reciprocal lattice and a TOF image taken after lattices are abruptly released. This TOF image is oriented such that its plane is orthogonal to the imaging light. (b) Two lattice ramp sequences used in this paper [25]. (c) A TOF image showing the first Brillouin zone.
FIG. 3. Interference patterns observed after we abruptly release scalar (top), LP spinor (middle), and TP spinor BECs (bottom) at various $u_L$ and a 5.5-ms TOF at $q_B/h = 360$ Hz. Panels (a)-(c) are taken after ramp-up sequences to a final $u_L = 2, 10$, and $26E_R$, respectively. Panels (d)-(e) are taken after ramp-down sequences to a final $u_L$ of $12E_R$ and $4E_R$. The field of view is $400\,\mu m \times 400\,\mu m$.

Distinct interference peaks can always be observed during ballistic expansion, after each of the three types of BECs is abruptly released from a shallow lattice of $u_L \leq 10E_R$. Here $E_R = h^2k^2_L/(8\pi^2M)$ is the recoil energy, $M$ and $h$ are respectively the atomic mass and the Planck constant, and $k_L$ is the lattice wave-vector (see Ref. [27]). As shown in the time of flight (TOF) images in Fig. 2(a) and Fig. 3, the six first-order diffracted peaks are symmetrically set apart from the central peak by a distance corresponding to a momentum of $2h k_L$ along three orthogonal axes. These interference peaks may be considered as an indicator for coherence associated with the SF phase in the system. In fact, a larger visibility of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD) of interference patterns, a narrower width of the central peak, and a higher optical density (OD).

As an example, the LP spinor BECs studied in Fig. 3 demonstrate long-range phase coherence at $u_L = 10E_R$ with a coherence length of around nine lattice sites, which is estimated from the ratio of the central peak width to $4h k_L$. Second, when $u_L$ is further increased and exceeds a critical value $u_c$, the interference peaks steadily smear out to a single broad peak indicating atoms completely lose phase coherence. We read off the value of $u_c$ in Fig. 4 from the intersection of two linear fits applied to the data of a given BEC. The loss of coherence can be accounted for by many mechanisms, such as heating, inelastic collisions, or entering into a MI state. To confirm the system has undergone a SF-MI transition, we monitor the lattice ramp-down sequence, because one characteristic of a MI state has proven to be a loss of phase coherence in deep lattices and a subsequent rapid revival of coherence as $u_L$ is reduced. As shown in Fig. 4(b), the interference peaks of both scalar and spinor BECs reversibly revive after the ramp-down sequences, indicating atoms quickly recohere and return to SF states.

Observations in Fig. 4 are qualitatively consistent...
with our MF calculations and suggest the existence of first-order SF-MI transitions under some circumstances. First, LP spinor BECs at high magnetic fields possess many properties (e.g., the peak OD) that are similar to those of scalar BECs. Their ramp-up and ramp-down curves are close to each other, while both have roughly symmetric transition points \( u_c \). Similar phenomena were observed in \(^{87}\text{Rb}\) and \(^{6}\text{Li}\) systems, and have been considered as signatures of second-order SF-MI transitions \([1, 2, 5]\). Second, LP states at low magnetic fields and TP states at high fields apparently have smaller \( u_c \) for both ramp-up and ramp-down processes compared to scalar BECs, suggesting enlarged Mott lobes. Particularly, the ramp-down \( u_c \) for LP states at low fields is noticeably smaller than their ramp-up \( u_c \), corroborating with the MF picture that hysteresis occurs across the first-order phase transitions. Third, the recovered interference contrast is visibly different for various BECs after the ramp-down process (after SF-MI phase transitions). For scalar and high-field LP spinor BECs, nearly 75\% of peak OD can be recovered in the interference peaks after the ramp-down sequence. The slightly reduced interference contrast may be due to unaccounted heating effects, which leads a small portion of atoms (<20\%) to populate the Brillouin zone. In contrast, after we utilized quite a few techniques and optimized many parameters, the maximal recovered interference contrast of low-field LP states is only \( \sim 40\% \) (\( \sim 20\% \) for high-field TP states). We attribute this to unavoidable heatings across the first-order transitions as there is a jump in system energy between meta-stable states and stable states. Both hysteresis effect and significant heatings strongly suggest that first-order SF-MI transitions are realized in our experiment. Note, however, we do not see noticeable jumps in the observables as it is typically associated with first-order transitions. This is likely due to the presence of even and odd atom fillings in inhomogeneous systems such as trapped BECs, although the predicted first-order SF-MI transitions only exist for even occupancy number. Limited experimental resolutions may be another reason.

In addition, our data of the LP state in Fig. 4(b) demonstrate the feasibility of realizing SF-MI transitions via a new approach, i.e., by ramping \( q_B \) at a fixed lattice depth. For example, when the final \( u_L \) in the ramp-down sequence is set at a value between \( 17E_R \) and \( 21E_R \), atoms in the LP spinor BECs can cross the SF-MI transitions if \( q_B \) is sufficiently reduced (e.g., from \( h \times 360 \) Hz to \( h \times 20 \) Hz). This agrees with the MF prediction in Fig. 4(d): \( u_c \) depends on \( q_B \) in antiferromagnetic spinor BECs.

We then compare scalar and spinor BECs within a wide range of magnetic fields, \( 20 \) Hz \( \leq q_B/h \leq 500 \) Hz, after identical lattice ramp sequences to \( u_L = 10E_R \). We choose \( 10E_R \) because it is apparently the lattice depth around which we observe the maximum interference contrast, with negligible difference in scalar and spinor BECs after the ramp-up sequence at all \( q_B \). This is consistent with Fig. 1 which predicts all BECs studied in this work should be well in the SF phase at \( 10E_R \). However, the interference peak ODs show intriguing differences after the ramp-down sequence to \( 10E_R \) (see Fig. 5): deviations from the maximal value appear for LP spinor BECs at low magnetic fields and the TP state at all positive \( q_B \). We again attribute this to different amount of heatings across the SF-MI transitions. Different extent of heatings may be produced due to different spin barriers as well as the amount of energy jump across the transitions. Hence, the maximum recovered OD is a good indicator for the appearance/disappearance of first-order phase transitions. Notably, LP spinor BECs are found to behave very similarly to scalar BECs as long as \( q_B \) is large enough, i.e., \( q_B \geq h \times 100 \) Hz > \( U_2 \) as shown in Fig. 4. This observation is again consistent with Fig. 4(d), in which the two MF curves for the LP state merge indicating that meta-stable states disappear and SF-MI transitions become second order when \( q_B/h > 70 \) Hz. Furthermore, the difference between LP and TP spinor BECs appears to exponentially decrease as \( q_B \) approaches zero. Exponential fits to the data verify that the LP and TP spinor BECs should show the same behavior at \( q_B = 0 \).

In conclusion, we have conducted the first experimental study on the SF-MI phase transitions in an antiferromagnetic sodium spinor BEC confined by 3D optical lattices. We have observed the hysteresis effect and significant heatings across the phase transitions, which suggest first-order SF-MI transitions are realized in our experiment. These observations and the dependence of the phase transitions on \( q_B \) can be qualitatively understood by MF theory. Further studies are required to confirm more signatures of the first-order transitions, for example by precisely imaging Mott shells \([12]\). Our data also suggest the feasibility of realizing SF-MI phase transitions via changing the quadratic Zeeman energy.
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\begin{align*}
S_{ix} &= \frac{\alpha}{\sqrt{5}} \left( b_{i,0}^\dagger b_{i,1} + b_{i,1}^\dagger b_{i,0} + b_{i,0}^\dagger b_{i,-1} + b_{i,-1}^\dagger b_{i,0} \right), \\
S_{iy} &= \frac{\alpha}{\sqrt{5}} \left( b_{i,1}^\dagger b_{i,0} - b_{i,0}^\dagger b_{i,1} + b_{i,-1}^\dagger b_{i,0} - b_{i,0}^\dagger b_{i,-1} \right), \\
S_{iz} &= b_{i,1}^\dagger b_{i,1} - b_{i,-1}^\dagger b_{i,-1}.
\end{align*}

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