Variational study of phase diagrams of spin–orbit coupled bosons

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Abstract
We use a variational order method to explore the ground state phase diagrams of spin–orbit coupled Bose atoms in optical lattices. By properly parameterizing the order with an ansatz function for each possible phase and comparing their energies which are minimized with respect to the variational parameters, we can effectively identify the lowest energy states and depict the phase diagram. While the Mott–insulator–superfluid phase boundary is computed by the usual Gutzwiller method, the spin-ordered phase structures of the deep Mott regime as well as the superfluid regime are studied by the variational order method. For the isotropic spin–orbit coupling, the phase diagram in the deep Mott insulator regime is qualitatively similar to results derived by the classical Monte-Carlo simulations or other numerical methods. The spiral phases with different spatial periods are discussed in detail. We also identify the uniform superfluid, stripe and checkerboard supersolid phases with exotic spin orders in the superfluid regime.

1. Introduction

The reversible tuning between Mott insulator (MI) and superfluid (SF) phases in ultracold atoms had been realized in the experiment by varying the strength of the periodic lattice potential [1, 2]. It is well known that low-energy properties can be described by the Bose–Hubbard model [3–14]. The model provides an ideal platform for the study of MI and SF phases, and the essence of the MI-SF phase transition. In the two-component Bose–Hubbard model, the magnetic phases are predicted in the limit of large repulsive interspecies interactions, such as the incompressible double-checkerboard solid and the supercounterflow [7–9]. On the other hand, the possibility of creating artificial gauge fields in the Bose–Einstein condensation (BEC) opens up a new era of the ultracold atom physics [15, 16]. Numerous ideas are proposed to generate artificial gauge fields, both Abelian and non-Abelian, with the prediction of many exotic properties in magnetic potentials and in optical lattices as well [17–30].

Combined with the controllability of interactions and geometries of ultracold bosons, the manipulation of spin–orbit coupling (SOC) gives rise to a lot of novel quantum states, especially the MI-SF phase transition and the magnetic orders in the deep MI and superfluid regimes [30–49]. For example, one can derive an effective super-exchange spin model with the Dzyaloshinskii–Moriya type (DM-type) interactions [50, 51] in the deep MI regime via the second-order perturbation theory. Some exotic spin textures are found by applying the classical Monte-Carlo (MC) simulations, the bosonic dynamical mean field theory (BDMFT) and the spin-wave theory [25–27, 39–42, 52]. The spiral superfluid phase in the vicinity of the MI-SF phase transition is discussed in [44, 45].

In this paper, we use a variational order method to explore the phase diagrams of SOC bosons in a square optical lattice. The spin orders of the ground state are non-uniform due to the SOC, so we parameterize each possible order with a proper ansatz function. By comparing the minimized energies of all phases with respect to the variational parameters, we effectively identify the lowest energy states and depict the phase diagram. While the MI-SF phase boundary is computed by the usual Gutzwiller method, the spin-ordered phase structures of the deep MI regime as well as the SF regime are studied by the variational order method. For the isotropic SOC,
the spiral (Sp), the vortex crystal (VX) and the skyrmion crystal (SkX) phases are found in the deep MI regime, which is qualitatively similar to the previous results derived from the classical MC simulations, the BDMFT and the spin–wave theory. The Sp phases with different spatial periods are discussed in detail. We further explore the phase diagrams in the MI regime with the anisotropic SOC and in the SF regime. Three new spin–ordered phases, namely, the pseudo-vortex (PVX), the helical (He) and the antiskyrmion (ASkX) crystal phases are found in the MI regime with the anisotropic SOC. We also identify the uniform superfluid (USF), the stripe supersolid (SSS) and the checkerboard supersolid (CSS) phases with exotic spin orders in the SF regime.

The paper is organized as follows: in section 2 we introduce the Bose–Hubbard model with Rashba-type SOC. In section 3 we compare the MI–SF phase diagram without and with the SOC by using the usual Gutzwiller mean-field theory. The spin–ordered phase diagrams in the deep MI and SF regimes are addressed respectively in section 4.1 and section 4.2 by the variational order method. A brief summary is included in section 5.

2. Model

The Hamiltonian of the two-species cold bosons in a square optical lattice is written as

$$\hat{H} = -t \sum_{\langle j,k \rangle} (\Phi_j^\dagger \Psi_{j} \Phi_k + \text{h.c.}) + \frac{1}{2} \sum_{j,\sigma} U_{\sigma \sigma'} \hat{b}^\dagger_{j \sigma} \hat{b}^\dagger_{j \sigma'} \hat{b}_{j \sigma'} \hat{b}_{j \sigma},$$

(1)

where $\hat{b}_{j \sigma}^\dagger$ ($\hat{b}_{j \sigma}$) is bosonic creation (annihilation) operator which creates (annihilates) a spin-$\sigma$ ($\sigma = \uparrow, \downarrow$) boson at site $j$. The operators are written as $\Phi_j^\dagger = (\hat{b}_{j \uparrow}^\dagger, \hat{b}_{j \downarrow}^\dagger)$ in equation (1). The first term of equation (1) describes tunneling of a boson between the neighboring sites $j$ and $i$ with the hopping amplitude $t$. The tunneling matrix $\Psi_{ji} \equiv \exp (i \hat{A} \cdot (\hat{r}_j - \hat{r}_i))$ with $\hat{A} = (\alpha \sigma_{xy} - \beta \sigma_x, 0)$ is the non-Abelian gauge field. The diagonal terms in the matrix denote the spin–conserved tunneling of the bosons whereas the off–diagonal terms denote the Rashba-type SOC which can be generated by a periodic pulsed magnetic field [22, 53–56]. The two-species bosons with SOC can be rewritten explicitly as

$$\hat{H} = -t \cos \alpha \sum_{\langle j,i \rangle,\sigma} (\hat{b}_{j \sigma}^\dagger \hat{b}_{i \sigma} + \text{h.c.}) - t \cos \beta \sum_{\langle j,i \rangle,\sigma} (\hat{b}_{j \sigma}^\dagger \hat{b}_{i \sigma} + \text{h.c.})$$

$$- t \sin \alpha \sum_{\langle j,i \rangle} \left( \hat{b}_{j \sigma}^\dagger \hat{b}_{i \sigma}^\dagger - \hat{b}_{j \sigma} \hat{b}_{i \sigma} \right) + \text{h.c.}$$

$$+ i t \sin \beta \sum_{\langle j,i \rangle} \left( \hat{b}_{j \sigma}^\dagger \hat{b}_{i \sigma}^\dagger + \hat{b}_{j \sigma} \hat{b}_{i \sigma} \right) + \text{h.c.}$$

$$+ \sum_{j,\sigma} \left[ \frac{U_{\sigma \sigma'}}{2} (n_{j \sigma} - 1) + U_{\sigma \sigma'} n_{j \sigma} n_{j \sigma'} - \mu_{\sigma} n_{j \sigma} - \mu_{\sigma'} n_{j \sigma'} \right].$$

(2)

Here $\sum_{\langle j,i \rangle} (\sum_{\langle j,i \rangle})$ represents summation over the neighboring sites in the $x(y)$ direction. $U_{\uparrow \downarrow} = U_{\downarrow \uparrow} = U$ and $U_{\uparrow \uparrow} = U_{\downarrow \downarrow} = gU$ are the intra-species and the interspecies interactions, respectively. $\alpha$ and $\beta$ are the SOC strengths of the $x$ and $y$ directions. In the context, we introduce a parameter $\lambda = \alpha / \beta$ to describe the symmetry of the SOC. The system size is $L \times L$ ($L = 12$) with periodic boundary conditions.

3. The MI–SF phase transition

In this section, we use the Gutzwiller method to investigate the MI–SF transition with the isotropic SOC ($\lambda = 1$). The wave function is given by [45]

$$|\Psi\rangle = \prod_j \left( \sum_{n_j n_j} C_{n_j n_j}^j |\psi_j\rangle \right),$$

(3)

where $|\psi_j\rangle = |n_j, n_j\rangle$ is the Fock state at site $j$ and the probability amplitudes $C_{n_j n_j}^j$ are, in general, complex and depend on the number of bosons at each site.
From equations (2) and (3), we obtain the energy functional

\[
E = \langle \Psi | H | \Psi \rangle = -t \cos \alpha \sum_{\langle ij \rangle, \sigma} (\Delta_{ij}^\sigma \Delta_{ij,\sigma} + \text{h.c.}) - t \cos \alpha \sum_{\langle ij \rangle, \sigma} (\Delta_{ij}^\sigma \Delta_{ij,\sigma} + \text{h.c.}) \\
- t \sin \alpha \sum_{\langle ij \rangle} (\Delta_{ij}^\dagger \Delta_{ij,\sigma} - \Delta_{ij,\sigma}^\dagger \Delta_{ij}^\dagger) + \text{h.c.} + it \sin \alpha \sum_{\langle ij \rangle} (\Delta_{ij}^\dagger \Delta_{ij,\sigma} + \Delta_{ij,\sigma}^\dagger \Delta_{ij}^\dagger) + \text{h.c.} \\
+ \sum_{n, \sigma} \sum_{n, \sigma} \left[ \frac{U}{2} (n_{j,\uparrow} - 1) + \mu_{\sigma} n_{j,\sigma} - (\mu_{\sigma} n_{j,\sigma} - g U n_{j,\sigma} - n_{j,\sigma}) \right] |C_{n,\sigma}^j|^2, 
\]

where

\[
\Delta_{ij} = \langle \Psi | \hat{b}_{j,\uparrow}^\dagger | \Psi \rangle = \sum_{n, \sigma} \sqrt{n_{j,\uparrow} + 1} C_{n,\sigma}^j C_{n+1,\sigma}^i, \\
\Delta_{ij}^\dagger = \langle \Psi | \hat{b}_{j,\downarrow}^\dagger | \Psi \rangle = \sum_{n, \sigma} \sqrt{n_{j,\downarrow} + 1} C_{n,\sigma}^{i\dagger} C_{n,\sigma}^{i+1}. 
\]

are the SF order parameters of spin-up and spin-down components, respectively. The SF order parameters are complex numbers in general and can be rewritten in terms of the magnitude and the phase, i.e., \( \Delta_{ij,\sigma} = |\Delta_{ij,\sigma}|e^{i\phi_{ij,\sigma}} \). Since \( U_{\uparrow\downarrow} = U_{\downarrow\uparrow} \) and \( \mu_\uparrow = \mu_\downarrow \), the order parameters \( \Delta_{ij} = \Delta_{ij} \). Due to the magnitudes of these parameters are uniform throughout the lattice while the phases vary from site to site \([44, 45]\), the SF order parameters are simplified as \( \Delta_{ij} = |\Delta|e^{i\phi_{ij}} \).

According to the definition of the \( \Delta_{ij,\sigma} \), the probability amplitudes also can be rewritten as

\[
C_{n}^{i\dagger} = |C_{n}^{i\dagger}|e^{i\phi_{n,i}}, \quad |C_{n}^{i\dagger}| = |C_{n}^{i\dagger}|e^{i\phi_{n,i}}, \quad \text{where} \quad \phi_{n,i} = \phi_{n,i}^{\uparrow} + \phi_{n,i}^{\downarrow}.
\]

The MI-SF phase transition can be determined by using the Gutzwiller method that minimizes the energy functional in equation (4). In figure 1, we display the difference of the phase boundaries without (\( \alpha = 0 \) in (a)) and with (\( \alpha = 0.2\pi \) in (b)) the SOC. The SOC frustrates the kinetic energy and reduces the bandwidth, therefore a larger bare hopping amplitude \( t \) is required at larger SOC to reach the SF phase.

### 4. Spin-ordered phases

We now investigate the spin-ordered phase diagrams in the deep MI and SF regimes respectively by using the variational order method. Due to the SOC, the spin-order of the ground state may be non-uniform and hence we parameterize the spin order by an ansatz function for each possible phase. By minimizing the energy functional with the variational parameters, we can obtain the lowest energy state as the ground state. In the following, we addressed the spin-ordered phase diagrams in the deep MI regime in 4.1 and the SF regime in 4.2, respectively. The details of the method are collected in the appendix.

#### 4.1. MI regime

In the deep MI regime (\( t/U = 0.01 \)) with commensurate filling, the spin fluctuations are determined by an effective magnetic Hamiltonian that is derived from the quantum perturbation theory. The effective Hamiltonian is written as \([25–27, 39–42]\).
Here, \( S_j = (S^x_j, S^y_j, S^z_j) \) are the spin operators of the bosons by definitions \( S^a_j = \frac{\Phi^\dagger a \Phi_j}{2} \) with \( \sigma^a(a = x, y, z) \) the Pauli matrices. The spin-coupling coefficients \( J^x_{ij} = -4t^2 \cos(2\alpha)/gU \), \( J^y_{ij} = -4t^2 \cos(2\alpha)/gU \), \( J^z_{ij} = J^z_{ij} = -4t^2(2g - 1) \cos(2\alpha)/gU \) and \( J^z_{ij} = J^z_{ij} = -4t^2(2g - 1) \cos(2\alpha)/gU \) represent the Heisenberg-type (H-type) super-exchange coupling strengths. \( D_\delta = -4t^2 \sin(2\alpha) \delta /U \) and \( D_\delta = 4t^2 \sin(2\alpha) \delta /U \) are the DM-type super-exchange coupling strengths, respectively.

The classical spin operator can be expressed by \( S_j = S(\sin \theta_\delta \cos \phi_\delta, \sin \theta_\delta \sin \phi_\delta, \cos \theta_\delta) \) in the spherical coordinate, with normalized length \( |S|^2 = 1 \). The energy functional \( E \) is obtained by substituting \( S_j \) into the \( H_{mag} \),

\[
E = \sum_{\langle j,k \rangle} [\sin \theta_{ij} \cos \phi_{ij} (\sin \theta_{ij} \cos \phi_{ij} J^x_{ij} - \cos \theta_{ij} |D_\delta|)] + \sum_{\langle j,k \rangle} [\sin \theta_{ij} \sin \phi_{ij} (\sin \theta_{ij} \sin \phi_{ij} J^y_{ij} + \cos \theta_{ij} \cos \theta_{ij} J^x_{ij} - \cos \theta_{ij} |D_\delta|)] + \sum_{\langle j,k \rangle} [\sin \theta_{ij} \sin \phi_{ij} (\sin \theta_{ij} \sin \phi_{ij} J^y_{ij} + \cos \theta_{ij} \cos \theta_{ij} J^x_{ij} - \cos \theta_{ij} |D_\delta|)] + \sum_{\langle j,k \rangle} [\sin \theta_{ij} \cos \phi_{ij} (\sin \theta_{ij} \cos \phi_{ij} J^x_{ij} - \cos \theta_{ij} |D_\delta|)].
\]

The phase diagrams of the deep MI regime are obtained by minimizing the energy \( E \) in equation (7) with respect to all possible macroscopic spin configurations. Due to the competition between the H-type and the DM-type super-exchange couplings, the xy-ferromagnetic (xy-FM), the z-ferromagnetic (z-FM), the z-antiferromagnetic (z-AFM), the Sp, the diagonal spiral phase (DSp) (with the spiral vector along the (11) or (1 Ī) direction), the 2 × 2 VX and the 3 × 3 SkX phases are found for the isotropic SOC (\( \lambda = 1 \)). The results are shown in figure 2(a). In the small \( \alpha \) region, the DM-type super-exchange coupling vanishes, the Hamiltonian reduces to the standard XXZ-Heisenberg model, where the H-type super-exchange coupling of the \( x - y \) in-plane component is larger than the \( z \)-component for \( g < 1 \), and vice versa. In the limit \( \alpha \rightarrow \pi/2 \), the case is identical to the small \( \alpha \). The H-type super-exchange along the \( x \) and \( y \) directions are of different signs which lead to the H-type super-exchange in spin-space has different sign for the \( x \) and \( y \) components and form the VX phase. The DM-type super-exchange coupling grows and the coplanar state becomes unstable, giving way to the SkX phases as \( \alpha \) reduces. The Sp phase results from the combination of the H-type super-exchange and the nonzero DM-type super-exchange in the intermediate values of SOC. Though the phase boundaries are not match well, the phase diagram is qualitatively similar to the previous result derived by the classical MC simulations, as the figure 2(a) in [25]. The various Sp phases with different spatial periods of \( n \) lattice sites (3 ≤ \( n \) ≤ 12) (called the Sp-n phase) are explicitly displayed in figure 2(b). We note that the spatial periods decrease with the increase of the SOC strength.

Figure 3 shows the ground state phase diagrams for the anisotropic SOC (\( \lambda \neq 1 \)). In contrast to the isotropic SOC, the 3 × 3 SkX and the Sp phases are replaced by the 3 × 3 ASkX and the 2 × 2 PVX phases for \( \lambda = 0.5 \). Here, the ASkX phase denotes that the spin at the center points to negative \( z \) direction while the spins away from the center tumble outward the positive \( z \) direction. The PVX phase denotes a non-coplanar state with \( \theta = \frac{\pi}{2} \). From figures 3(a) and (b), one observes that the anisotropic SOC leads to a sequence of transitions from the z-FM phase to the 3 × 3 ASkX phase, and to the 2 × 2 PVX phase for increasing strength \( \alpha \). Figures 3(c) and (d) reveal a He phase in which the spins at the odd number of lattice sites point to the negative \( z \) direction and those
at the even number lattice sites pose a spiral pattern for $\lambda = 5$. Due to the symmetry of DM-type super-exchange and the coplanar feature of the system are broken, the $3 \times 3$ ASkX, the $2 \times 2$ PVX and the He phases are found in the anisotropic SOC system.

4.2. SF regime

In the SF regime, the wave functions of the two-component bosons are characterized in terms of the four parameters $(\rho_j, \phi_j, \theta_j, \varphi_j)$,

$$
\Psi_j = \left( \begin{array}{c} \psi_{j,\uparrow} \\ \psi_{j,\downarrow} \end{array} \right) = \sqrt{\rho_j} e^{i\phi_j} \left( \cos \left( \frac{\alpha}{2} \right) e^{-i\eta_j/2} \right) \sin \left( \frac{\alpha}{2} \right) e^{i\eta_j/2},
$$

(8)

where $\rho_j$ and $\phi_j$ are the density and phase at site $j$ with normalization $\sum_j \rho_j = 1$. Substituting equation (8) into equation (2) gives rise to the energy functional

$$
E = -t \cos \alpha \sum_{(j,k),\sigma} (\Psi^\dagger_{j,\sigma} \Psi_{k,\sigma} + \text{H.c.}) - t \cos (\lambda \alpha) \sum_{(j,k),\sigma} (\Psi^\dagger_{j,\sigma} \Psi_{k,\sigma} + \text{H.c.}) - t \sin \alpha \sum_{(j,k)} (\Psi^\dagger_{j,\uparrow} \Psi_{k,\downarrow}

- \Psi^\dagger_{j,\downarrow} \Psi_{k,\uparrow}) + \text{h.c.} + \text{it} \sin (\lambda \alpha) \sum_{(j,k)} (\Psi^\dagger_{j,\uparrow} \Psi_{k,\downarrow} + \Psi^\dagger_{j,\downarrow} \Psi_{k,\uparrow}) + \text{h.c.} + \sum_{j,\sigma} \left( \frac{U}{2} |\Psi_{j,\sigma}|^4 + gU |\Psi_{j,\sigma}|^2 |\Psi_{j,\sigma'}|^2 \right).
$$

(9)

The ground state phase diagrams of the SF regime are obtained by minimizing the $E$ in equation (9) with respect to various configurations of the parameters $(\rho_j, \phi_j, \theta_j, \varphi_j)$. For the isotropic SOC, four types of phases are found in figure 4. These phases are the USF phase with xy-FM order (USF-xy-FM), the USF phase with Sp order with spatial period of 3 lattice sites (USF-3-3), the SSS phase with Sp order with spatial period of 12 lattice sites (SSS-3x3), and the USF phase with $2 \times 2$ spin VX order (USF-2x2-VX).

Figure 5 displays the spin-ordered phase diagrams for the anisotropic SOC system. Except the phases revealed in figure (4), we observe the SSS phases with $2 \times 2$ spin VX order (SSS-2x2-VX), the xy-FM order (SSS-xy-FM), the He order with spatial period of 12 lattice sites (SSS-He-12), and the USF phase with $3 \times 3$ SkX order (USF-3x3-SkX). In figure 5(c), a CSS phase of He order with spatial period of 12 lattice sites (CSS-He-12) appears. In certain regions, the USF, the SSS and the CSS phases with exotic spin orders are preferred since they have the lowest energies.
5. Summary

We have used a variational order method to study the ground state phase diagrams in the deep MI and the SF regimes for the SOC bosons in the optical lattice. In the deep MI regime, the Sp, the VX and the SkX phases are found for the isotropic SOC system. Three new spin-ordered phases, the PVX, the He and the ASkX phases appeared for the anisotropic SOC system. We also identify the USF, the SSS and the CSS phases with exotic spin-order in the SF regime. Our method is effective to deal with such systems and can provide clues to search the various magnetic phases in the ultracold atom experiment. The method also can be extended to other optical lattices and to higher dimensional spaces.

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Appendix. Variational method

In the deep MI regime, the parameters \((\theta_j, \varphi_j)\) can be parameterized by the a distribution function. For example, in the Sp-\(n\) phase we suppose that

\[
\begin{align*}
\theta_j &= \hat{j}_x \alpha + \hat{j}_y \beta + \psi, \\
\varphi_j &= \hat{j}_x \gamma + \hat{j}_y \eta + \phi,
\end{align*}
\]

where \((\alpha, \gamma)\) and \((\beta, \eta)\) are the azimuthal angles along the \(x\) and \(y\) directions at site \(j = (\hat{j}_x, \hat{j}_y)\). \(\psi\) and \(\phi\) are the regulation parameters for the different lattice sites. The parameters \((\alpha, \gamma, \beta, \eta, \psi, \phi)\) are determined by the spin configurations of the possible phases. By minimizing the energy \(E\) in equation (7) with respect to variational parameters, we get \(\alpha = \gamma = \eta = \psi = 0\) and \(\beta = \frac{\pi}{n}\). For \(n\) even number, one has

Figure 4. Spin-ordered phase diagrams in the SF regime at the isotropic SOC bosons for different values of \(t/U\): (a) \(t/U = 0.05\), (b) \(t/U = 0.1\), and (c) \(t/U = 1\).

Figure 5. Spin-ordered phase diagrams in the SF regime for the anisotropic SOC bosons at fixed \(t/U = 0.1\): (a) \(\lambda = 0\), (b) \(\lambda = 0.5\), and (c) \(\lambda = 2\)
The energy reaches the minimum value as the variational parameters
\[
\phi = \frac{\pi}{2}, \quad 1 \leq j_y \leq \frac{n}{2},
\]
\[
\phi = \frac{3\pi}{2}, \quad \frac{n}{2} < j_y \leq n,
\] (A2)
while for \(n = \text{odd number},\)
\[
\phi = \frac{\pi}{2}, \quad 1 \leq j_y < \frac{n + 1}{2},
\]
\[
\phi = 0, \quad j_y = \frac{n + 1}{2},
\]
\[
\phi = \frac{3\pi}{2}, \quad \frac{n + 1}{2} < j_y \leq n.
\] (A3)
For the \(n \times n\) SkX phase \((n = \text{odd number}),\) the parameters take
\[
\theta_j = \alpha \left( j_x - \frac{n + 1}{2} \right) + \left( j_y - \frac{n + 1}{2} \right)^2,
\] (A4)
and
\[
\varphi_j = \beta \left( j_x + j_y - 1 \right), \quad 1 \leq j_x < \frac{n + 1}{2}, \quad 1 \leq j_y \leq n,
\]
\[
\varphi_j = 2\pi - \beta \left( j_x + j_y - n \right), \quad \frac{n + 1}{2} \leq j_x \leq n, \quad 1 \leq j_y \leq n.
\] (A5)
The energy reaches the minimum value as the variational parameters \(\alpha = \frac{\pi}{2}\) and \(\beta = \frac{\pi}{4}\), \(n = 3\), which is the \(3 \times 3\) SkX phase. All other phases in the deep MI regime are obtained by these processes. The phase diagrams in the SF regime are obtained by similar processes.

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