Spin-orbit coupled repulsive Fermi atoms in a one-dimensional optical lattice

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Abstract
Motivated by recent experimental development, we investigate spin–orbit coupled repulsive Fermi atoms in a one-dimensional optical lattice. Using the density-matrix renormalization group method, we calculate the momentum distribution function, gap, and spin-correlation function to reveal rich ground-state properties. We find that spin–orbit coupling (SOC) can generate unconventional momentum distribution, which depends crucially on the filling. We call the corresponding phase with zero gap the SOC-induced metallic phase. We also show that SOC can drive the system from the antiferromagnetic to ferromagnetic Mott insulators with spin rotating. As a result, a second-order quantum phase transition between the spin-rotating ferromagnetic Mott insulator and the SOC-induced metallic phase is predicted at the strong SOC. Here spin rotating means the spin orientations of the nearest-neighbor sites are not parallel or antiparallel, i.e., they have an intersection angle \( \theta \in (0, \pi) \). Finally, we show that the momentum \( k_{\text{peak}} \), at which the peak of the spin-structure factor appears, can also be affected dramatically by SOC. The analytical expression of this momentum with respect to the SOC strength is also derived, which suggests that the predicted spin-rotating ferromagnetic (\( k_{\text{peak}} < \pi / 2 \)) and antiferromagnetic (\( \pi / 2 < k_{\text{peak}} < \pi \)) correlations can be detected experimentally by measuring the SOC-dependent spin-structure factor via time-of-flight imaging.

1. Introduction

Ultracold Fermi atoms in optical lattices have attracted considerable interest both experimentally [1–16] and theoretically [17–41], because these setups are powerful platforms to simulate rich physics of strongly-correlated materials [42, 43]. One of advantages of this system is that the spatial geometry of optical lattices can be well controlled. In particular, using a strong harmonic transverse confinement, one-dimensional (1D) optical lattices have been achieved experimentally [2, 9]. On the other hand, the relative parameters have high controllability, and moreover, can reach the regimes that are not accessible to conventional condensed-matter physics. For example, the two-body interaction between Fermi atoms can be tuned by a magnetic-field-dependent Feshbach resonant technique [44], and thus ranges from the positive (repulsive) to the negative (attractive). For the on-site repulsive interaction, a well-known second-order quantum phase transition between an antiferromagnetic Mott insulator and a metallic phase can emerge [45].

Another important breakthrough in recent experiments of ultracold Fermi atoms is successfully creating a synthetic spin–orbit coupling (SOC), with equal Rashba and Dresselhaus strengths, using a pair of counter-propagating Raman lasers [46–49]. Indeed, SOC describes the interaction between the spin and orbit degrees of freedom of a particle. In contrast to the typical property of solid-state materials where the intrinsic SOC strength is generally smaller than the Fermi velocity of electrons, the synthetic SOC strength realized here can reach the same order as (or even larger than) the Fermi velocity of atoms, and moreover, can also be tuned in a wide range [50, 51]. Recent theory has revealed that SOC can generate exotic superfluids, including topological Bardeen–Cooper–Schrieffer [52–59] and topological Fulde–Ferrell–Larkin–Ovchinnikov [60–62] phases for the
attractive Fermi atoms. The fundamental idea for achieving these nontrivial topological superfluids is that the SOC, Zeeman field, and s-wave interaction can induce triplet p-wave pairing \[63–65\]. In parallel with the attractive case, it is natural to ask what novel physics can occur in the repulsive Fermi atoms driven by the synthetic SOC \[66–68\].

Inspired by the above experimental developments and theoretical considerations, here we investigate SOC repulsive Fermi atoms in a 1D optical lattice. Recently, spin–orbit coupled Bose–Einstein condensates in the 1D optical lattice were prepared experimentally \[69\]. Using a similar technique, the system considered here could also be achieved in the near future. Physically, the spin–orbit coupled Fermi atoms in the optical lattices have two characteristics. One is that SOC can make Fermi atoms hop between the nearest-neighbor sites with spin flipping (see the Hamiltonian \(\text{(6)}\) in the following). Moreover, it has strong competition with the on-site repulsive interaction, and in particular, with the conventional spin-independent hopping (see the Hamiltonian \(\text{(4)}\) in the following). The other is that in the presence of SOC, for different chemical potentials, the fillings are quite different (see figure 1).

Notice that in 1D quantum fluctuation becomes significant, and the mean-field results are, in principle, unreliable \[70\]. Here we capture the required ground-state properties, including momentum distribution and spin-correlation, by using the density-matrix renormalization group (DMRG) method \[71, 72\], which is a powerful numerical method to study lower-dimensional strong-correlated systems \[73\]. The main results are given as follows. Section 2 is devoted to introducing our proposal and deriving a 1D Fermi-Hubbard model with the synthetic SOC. Section 3 is devoted to addressing the generalized results without the on-site repulsive interaction. In this section, the unconventional momentum distribution, which depends crucially on the filling, is found. We call the corresponding phase the SOC-induced metallic phase. Section 4 is devoted to discussing the results in the presence of the on-site repulsive interaction. By means of the spin-correlation function, we find that SOC can drive the system from a spin-rotating antiferromagnetic Mott insulator to a spin-rotating ferromagnetic Mott insulator. As a result, a second-order quantum phase transition between the spin-rotating ferromagnetic Mott insulator and the SOC-induced metallic phase is predicted at the strong SOC. Here spin rotating means the spin orientations of the nearest-neighbor sites are not parallel or antiparallel, i.e., they have an intersection angle \(\theta \in (0, \pi)\) (see figure 8 in the following). In the spin-rotating antiferromagnetic Mott

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**Figure 1.** Spin–orbit coupled energy bands in an optical lattice and the corresponding fillings for different chemical potentials. The blue arrows represent spin polarizations in different subbands. The red dots denote the contact points of two subbands. \(k_{\text{min}}\) and \(k_{\text{max}}\) are the minimum and maximum of subbands, and are determined by equations \(\text{(12)}\) and \(\text{(13)}\), respectively, if the on-site repulsive interaction is not taken into account. (a) and (b) show the fillings for the small chemical potentials. In these cases, only the lower subband (the black shadow) is partly occupied. In (a), there are four Fermi points and no occupation around \(k = 0\) occurs, while in (b) there are three Fermi points and the occupation at \(k = 0\) emerges. (c) and (d) show the fillings for the large chemical potentials, in which the occupations in both the lower and upper (the red shadow) subbands emerge. In (c), the lower subband is still partly occupied, while in (d), the lower subband is fully occupied for a larger chemical potential.
insulator, $\pi/2 < \theta < \pi$, the quasi-long-range spin correlation decays as a power law and changes the sign with a period $2 < T < 4$, whereas for the spin-rotating ferromagnetic Mott insulator, $\theta < \pi/2$, the quasi-long-range spin correlation also decays as a power law but with the period $T > 4$. Finally, we show that the momentum $k_{\text{peak}}$, at which the peak of the spin-structure factor appears, can also be affected dramatically by SOC. The analytical expression of this momentum with respect to the SOC strength is also derived, which suggests that the predicted spin-rotating ferromagnetic ($k_{\text{peak}} < \pi/2$) and antiferromagnetic ($\pi/2 < k_{\text{peak}} < \pi$) correlations can be detected experimentally by measuring the SOC-dependent spin-structure factor via time-of-flight imaging [74]. The discussions and conclusions are given in section 5.

2. Model and Hamiltonian

2.1. Proposed experimental setup

Figure 2 shows our theory that repulsive Fermi atoms in a 1D optical lattice are driven by a pair of counter-propagating Raman lasers. For the specific experiments, 3D optical lattice is first prepared by the interference of three pairs of counter-propagating laser beams [42, 43]. The corresponding periodic potential can be written as

$$V_{\text{3D}} = V_0 \cos(k_y x) + V_0 \cos(k_x y) + V_0 \cos(k_z z),$$

where $V_0$ is the lattice depth, $k_y = 2\pi/\lambda_w$ is the wave vector, and $\lambda_w$ is the wavelength. By further using a strong harmonic transverse confinement $V = m_0\omega_t^2 r^2/2$ in the 3D optical lattice, i.e., where the 2D harmonic potential frequency $\omega_t$ is far larger than the trapping frequency $\omega_z$ along the weakly-confining axis, the required 1D optical lattice can be generated [2, 9] (see figure 2(a)). In such case, the two-body interaction between Fermi atoms is described effectively by [75]

$$U(z) = -\frac{2\hbar^2}{m_0} a_{\text{1D}} \delta(z),$$

with the 1D $s$-wave scattering length

$$a_{\text{1D}} = -\frac{a_t^2}{2a_{\text{3D}}} \left(1 - C\frac{a_{\text{3D}}}{a_t}\right),$$

where $C \approx 1.46$, $a_t = (2\hbar/m_0\omega_t)^{1/2}$, $a_{\text{3D}}$ is the 3D $s$-wave scattering length, and $m_0$ is the atomic mass. In addition, the pair of counter-propagating Raman lasers shown in figure 2(b) are used to create the required 1D synthetic SOC, with equal Rashba and Dresselhaus strengths [76]. In this method, the corresponding two spin states are chosen as $\left| \uparrow \right> = \left| 9/2, -9/2 \right>$ and $\left| \downarrow \right> = \left| 9/2, -7/2 \right>$ for a $^{40}$K system [46], or $\left| \uparrow \right> = \left| 3/2, -3/2 \right>$ and $\left| \downarrow \right> = \left| 3/2, -1/2 \right>$ for a $^6$Li system [49] (see figure 2(c)).

2.2. Hamiltonian

The total dynamics illustrated by figure 2 are governed by the following 1D Fermi–Hubbard model with the synthetic SOC [71, 72]:

![Figure 2. (a) Proposed experimental setup for realizing spin–orbit coupled repulsive Fermi atoms (FA) in a 1D optical lattice. (b) The interaction between FA and a pair of counter-propagating Raman lasers, labeled R1 and R2, respectively. These Raman lasers create a momentum-sensitive coupling between two internal atomic states, i.e., a synthetic SOC with equal Rashba and Dresselhaus strengths. (c) Energy levels and their transitions are induced by Raman lasers.](image-url)
H = H_i + H_u + H_{soc} \tag{3}

with

\begin{align}
H_i &= -t \sum_{l, \sigma = \uparrow, \downarrow} \left( c_{l \sigma}^\dagger c_{l+1 \sigma} + \text{H. c.} \right), \tag{4} \\
H_u &= U \sum_{l} n_{l \uparrow} n_{l \downarrow}, \tag{5}
\end{align}

and

\begin{align}
H_{soc} &= \lambda \sum_{l} \left( c_{l \uparrow}^\dagger c_{l+1 \uparrow} - c_{l \downarrow}^\dagger c_{l+1 \downarrow} + \text{H. c.} \right), \tag{6}
\end{align}

where \( c_{l \sigma}^\dagger \) and \( c_{l \sigma} \) are the creation and annihilation operators, with spin \( \sigma = \uparrow, \downarrow \), at lattice site \( l \). \( n_{l \sigma} = c_{l \sigma}^\dagger c_{l \sigma} \) is the number operator, \( t \) is the spin-independent hopping magnitude, \( U \) is the on-site repulsive interaction strength, and \( \lambda \) is the SOC strength. Based on the above proposal experimental setups, the relative parameters can be tuned independently. For example, the hopping magnitude \( t \) can be controlled by the intensities of lasers \([42, 43] \), the 1D on-site repulsive interaction strength \( U \) can be tuned by Feshbach resonance \([44] \), and the SOC strength \( \lambda \) can be driven through a fast and coherent modulation of Raman lasers \([50, 51] \). As a consequence, for a proper optical lattice, the SOC strength \( \lambda \) has the same order of the hopping magnitude \( t \) \([77] \).

2.3. Momentum distribution and spin correlation

In terms of the SOC-induced properties (see Introduction), here we mainly focus on momentum distribution and spin correlation, which can be measured experimentally by the time-of-flight imaging \([4, 15, 46, 74] \). The momentum distribution functions for spin-up and spin-down atoms are written, respectively, as \([78] \)

\begin{align}
n_{\uparrow}(k) &= \frac{1}{L} \sum_{lj} e^{i(k-l)j} \left( c_{l \uparrow}^\dagger c_{j \uparrow} \right), \tag{7} \\
n_{\downarrow}(k) &= \frac{1}{L} \sum_{lj} e^{i(k-l)j} \left( c_{l \downarrow}^\dagger c_{j \downarrow} \right). \tag{8}
\end{align}

For the Hamiltonian (3), the spin-up and spin-down atoms are equal, which means that \( n_{\uparrow}(k) \) is the same as \( n_{\downarrow}(k) \), and thus we only consider \( n_{\uparrow}(k) \) in the following discussions. The spin-correlation function is defined as \([74, 78, 79] \)

\begin{align}
S(r) &= \frac{1}{L} \sum_{lj} \left( s_l^x s_{l+r}^x \right), \tag{9}
\end{align}

where \( r \) is a distance between different sites and \( s_l^x = c_{l \uparrow}^\dagger c_{l \downarrow} - c_{l \downarrow}^\dagger c_{l \uparrow} \). The corresponding spin-structure factor is given by \([74, 78, 79] \)

\begin{align}
S(k) &= \frac{1}{L} \sum_{lj} e^{i(k-l)j} \left( s_l^x s_j^x \right). \tag{10}
\end{align}

Since the spin-structure factor has the sum extending over all lattice sites \( l \) and \( j \), it reflects spin correlation globally, and is thus used experimentally to detect the magnetic order \([74] \).

In addition, we will perform the DMRG calculations, with open boundary condition, to calculate equations (7)–(10). The basic energy scale is chosen as \( t = 1 \). In the detailed calculations, we retain 150 truncated states (which is sufficient) per DMRG block and 20 sweeps with the maximum truncation error \( \sim 10^{-5} \) \([80, 81] \).

3. Without on-site repulsive interaction

In order to better understand the fundamental physics induced by SOC, we first consider a simple case without the on-site repulsive interaction \( (U/t = 0) \) in which the Hamiltonian (3) reduces to \( H_i = H_{i} + H_{soc} \), i.e.,

\begin{align}
H_i &= -t \sum_{l, \sigma = \uparrow, \downarrow} \left( c_{l \sigma}^\dagger c_{l+1 \sigma} + \text{H. c.} \right) + \lambda \sum_{l} \left( c_{l \uparrow}^\dagger c_{l+1 \uparrow} - c_{l \downarrow}^\dagger c_{l+1 \downarrow} + \text{H. c.} \right). \tag{11}
\end{align}

In experiments, the 1D non-interacting Fermi atoms can be realized by tuning the 3D \( s \)-wave scattering length \( a_{3D} \) to its zero crossing. In such case, the 1D \( s \)-wave scattering length \( a_{1D} \to \infty \), and the 1D effective two-body interaction \( U(z) \) then becomes zero \([6, 7, 43] \) (see equations (1) and (2)).

3.1. Momentum distribution function

In the absence of SOC \( (\lambda/t = 0) \), the system has three known features. First, the energy bands of the Hamiltonian \( H_i \) are degenerate, and the system is located at the metallic phase. Secondly, all Fermi atoms occupy the degenerate energy bands from \( k_{min} = 0 \), where \( k_{min} \) is the minimum of the energy bands. Moreover, there are
two degenerate Fermi surfaces at the Fermi momentum $k_F = \pi / 2$, with filling factor $n = N/L$, where $N$ is the total atomic number. Lastly, the chemical potential cuts the degenerate energy bands with the Fermi momenta $\pm k_F$. As a result, the momentum distribution function $n_\uparrow(k)$ has a plateau of 1, with sharp edges at $k = \pm k_F$ (see the black solid curve of figure 3(a)). In the large-$k$ limit, this plateau of 1 disappears and two plateaus of 0 emerge, as expected. For the different chemical potentials, the fillings are similar, and the momentum distributions are thus similar (see the black solid curves of figures 3(b) and (c)).

In the presence of SOC $(\lambda / t \neq 0)$, the results are very interesting. In this case, the energy bands governed by the Hamiltonian $H_1$ split into two non-degenerate subbands, whose minima and maxima are given respectively by

$$k_{\text{min}} = \pm 2 \arctan \left( \frac{-t + \sqrt{t^2 + \lambda^2}}{\lambda} \right)$$

$$k_{\text{max}} = \pm 2 \arctan \left( \frac{t + \sqrt{t^2 + \lambda^2}}{\lambda} \right)$$

It is easy to find that $k_{\text{min}} + k_{\text{max}} = \pi$. For $\lambda = 0$, $k_{\text{min}} = 0$, as expected. In the presence of SOC $(\lambda \neq 0)$, there are generally four Fermi points when the chemical potential cuts two nondegenerate subbands. If the chemical potential is identical to the critical chemical potential $\bar{\mu}$ that just cuts the contact point (see the blue curve in figure 1(b)), three Fermi points can emerge. More importantly, for the different chemical potentials, the fillings are quite different (see figure 1). These different fillings affect dramatically the momentum distributions. As examples, we plot, in figure 3, the momentum distribution functions $n_\uparrow(k)$ for the different SOC strengths $\lambda / t$ when the filling factors are chosen as (a) $n = 0.3$, (b) $n = 1$, and (c) $n = 1.7$.

It can be seen from figure 3(a) that for a smaller filling, any SOC leads to a new momentum distribution in which the corresponding function $n_\uparrow(k)$ has two plateaus of 1/2, apart from the conventional plateau of 1. The physical explanation is given as follows. When the SOC strength is not strong enough (see, e.g., $\lambda / t = 0.2$), $\mu > \bar{\mu}$, and thus both the lower and upper subbands are partly occupied (see figure 1(c)). The occupation in the upper subband determines the plateau of 1, while the occupation in the lower subband governs two plateaus of 1/2. With the increase of the SOC strength $\lambda / t$, i.e., the chemical potential $\mu$ decreases [83, 84], the occupation
in the upper subband becomes less, and thus the width of the plateau of 1 becomes narrower. In particular, when \( \lambda / t = 0.52 \), the plateau of 1 disappears, since in this case \( \mu = \bar{\mu} \), and thus no occupation in the upper subband can be found. When further increasing the SOC strength \( \lambda / t \), i.e., \( \mu < \bar{\mu} \), a plateau of 0 emerges around \( k = 0 \) (not in the large-\( k \) limit). This is because there is no occupation around \( k = 0 \) when \( \mu < \bar{\mu} \) (see figure 1(a)). For the half filling (\( n = 1 \)), we find that the momentum distribution function \( n_1(k) \) usually has two plateaus of 1 and \( 1/2 \) (see figure 3(b)), because \( \mu > \bar{\mu} \) and both the lower and upper subbands are partly occupied. For a larger filling factor (see, e.g., \( n = 1.7 \)), the momentum distribution function \( n_1(k) \) has two plateaus of 1 and \( 1/2 \) when \( \lambda / t = 2.0 \) (see figure 3(c)). In this case, \( \mu > \bar{\mu} \) and the lower subband is totally occupied with a part occupation in the upper subband (see figure 1(d)). This case cannot occur in the smaller filling factors. We call the corresponding phase, with the above unconventional momentum distributions, the \textit{SOC-induced metallic phase}. Finally, in order to see clearly the above evolution of momentum distribution with respect to the filling factor, we plot the momentum distribution functions \( n_1(k) \) for the different filling factors \( n \) in figure 3(d).

It should be noted that in the case with a Zeeman field, but without the SOC, the chemical potential cutting the Zeeman-split bands also results in more than two Fermi points. However, the momentum distribution function \( n_1(k) \) is quite different from that induced by SOC. In such case, the momentum distribution function \( n_1(k) \) only has a plateau of 1. Moreover, for the different chemical potentials, the fillings are similar, and thus the momentum distribution functions \( n_1(k) \) are also similar. However, in our considered case with SOC, but without the Zeeman field, the momentum distribution function \( n_1(k) \) has the new plateaus of 1 for the different SOC strengths \( \lambda / t \), see figures 4(a) and (b). For the different SOC strengths \( \lambda / t \), see figure 3(d), the filling factor, we call the corresponding phase, with the above unconventional momentum distributions, the \textit{SOC-induced metallic phase}. Finally, in order to see clearly the above evolution of momentum distribution with respect to the filling factor, we plot the momentum distribution functions \( n_1(k) \) for the different filling factors \( n \) in figure 3(d).

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### 3.2. Spin–correlation function and spin–structure factor

Since SOC can make Fermi atoms hop between the nearest-neighbor sites, with spin flipping (see figure 2(a) and the Hamiltonian (6)), it is in competition with the conventional spin-independent hopping. This competition has a strong effect on the spin distributions of different sites. To see this clearly, we consider the spin–correlation function in equation (9)).

In figures 4(a) and (b), we plot the spin correlations between the nearest-neighbor sites, i.e., \( \langle \hat{S}_i^z \hat{S}_{i+1}^z \rangle \), and the next-nearest-neighbor sites, i.e., \( \langle \hat{S}_i^z \hat{S}_{i+2}^z \rangle \), respectively. These two subfigures show clearly that in the absence of SOC (\( \lambda / t = 0 \)), \( \langle \hat{S}_i^z \hat{S}_{i+1}^z \rangle < 0 \) and \( \langle \hat{S}_i^z \hat{S}_{i+2}^z \rangle = 0 \), which means that this short-range spin correlation is negative. In the presence of SOC (\( \lambda / t \neq 0 \)), the spin correlation is still short range. Interestingly, with the increase of the SOC strength \( \lambda / t \), the spin correlation varies from the negative to the positive at the critical point \( \lambda / t = 1 \). The physical reason will be illustrated in the following section.

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*Figure 4. Spin correlations between (a) the nearest-neighbor sites, i.e., \( \langle \hat{S}_i^z \hat{S}_{i+1}^z \rangle \), and (b) the next-nearest-neighbor sites, i.e., \( \langle \hat{S}_i^z \hat{S}_{i+2}^z \rangle \), for the different SOC strengths \( \lambda / t \). (c) The spin-structure factors \( S(k) \) for the different SOC strengths \( \lambda / t \). In all subfigures, the filling factor, the on-site repulsive interaction strength, and the lattice length are given by \( n = 1 \), \( U = 0 \), and \( L = 100 \), respectively.*
We now consider the case with the on-site repulsive interaction. With on-site repulsive interaction, the difference between the energy required to add a Fermi atom from the ground state. In the absence of SOC, the system is always located at the antiferromagnetic Mott insulator and the SOC-induced metallic phase at the half filling. In the following, we will show that SOC can drive the system from the antiferromagnetic to the ferromagnetic Mott insulator.

**4. With on-site repulsive interaction**

We now consider the case with the on-site repulsive interaction \( U/t > 0 \). In the absence of SOC \( \lambda/t = 0 \), it has been demonstrated exactly that for the 1D homogeneous Fermi–Hubbard model at the half filling \( n = 1 \), the metallic phase occurs at \( U = 0 \). For \( U > 0 \), the system is always located at the antiferromagnetic Mott insulator \([45]\), in which the spin orientations of the nearest-neighbor sites are antiparallel \([78]\), which means that a second-order quantum phase transition between the metallic phase and the antiferromagnetic Mott insulator emerges at \( U = 0 \). In the following, we will show that SOC can drive the system from the antiferromagnetic to the ferromagnetic Mott insulators with spin rotating (i.e., the spin orientations of the nearest-neighbor sites are not parallel or antiparallel), and predict a second-order quantum phase transition between the spin-rotating ferromagnetic Mott insulator and the SOC-induced metallic phase at the half filling \( n = 1 \).

**4.1. Momentum distribution function and gap**

Figures 5(a) and (d) show the momentum distribution functions \( n_\lambda(k) \) for the different SOC strengths \( \lambda/t \) at the half filling \( n = 1 \). In the absence of SOC \( \lambda/t = 0 \) and the on-site repulsive interaction strength \( U/t = 0 \), the momentum distribution function \( n_\lambda(k) \) has two sharp edges at \( k = \pm k_F \) (see the black solid curve in figure 5(a)). When increasing the on-site repulsive interaction strength \( U/t \), the momentum distribution functions \( n_\lambda(k) \) become smoother and all sharp edges disappear. In order to see the relevant physics more clearly, we introduce the gap \([45]\)

\[
\Delta = \mu^+ - \mu^-,
\]

where \( \mu^+ = E_g(N+1) - E_g(N) \) and \( \mu^- = E_g(N) - E_g(N-1) \), with the ground-state energy \( E_g \). This gap reflects the difference between the energy required to add \( \mu^+ \) and remove \( \mu^- \) a Fermi atom from the ground state. In the thermodynamic limit \( L \to \infty \), it has been demonstrated rigorously that \( \Delta \equiv 0 \) for \( U/t = 0 \) and \( \Delta \neq 0 \)
for $U/t > 0$. Moreover, $\Delta \equiv 0$ corresponds to the metallic phase and $\Delta = 0$ corresponds to the Mott insulator [45]. In our numerical results, due to finite-size effects, the gap is not absolute zero when $U/t = 0$ (see figure 5(b)). However, this result can be extrapolated to the thermodynamical limit by finite-size-scaling analysis [85, 86]. As shown in figure 5(c), we find $\Delta \equiv 0$ for $U/t = 0$ and $\Delta = 0$ for $U/t > 0$ in the thermodynamical limit. Therefore, here we call the phase in which $n_i (k)$ has sharp edges at $k = \pm k_2$ and $\Delta \equiv 0$ (thermodynamical limit), the metallic phase, whereas the phase in which $n_i (k)$ become smoother, all sharp edges disappear, and $\Delta = 0$ (thermodynamical limit) is referred to as the Mott insulator [45]. Since in this Mott insulator the spin orientations of the nearest-neighbor sites are antiparallel, the phase is finally called the antiferromagnetic Mott insulator (see also the following discussions).

In the presence of SOC (see, e.g., $\lambda / t = 1$), the momentum distribution function $n_i (k)$ is unconventional and $\Delta \equiv 0$ (thermodynamical limit), when $U/t = 0$ (see the black solid curve in figures 5(d)–(f)), which implies that the system is located at the SOC-induced metallic phase. When increasing the on-site repulsive interaction strength $U/t$, these momentum distribution functions $n_i (k)$ also become smoother, all sharp edges also disappear, and $\Delta = 0$ (thermodynamical limit), i.e., the system enters into the Mott insulator. However, as will be shown in the next subsection, these Mott insulators, without SOC or with SOC, are quite different. Without SOC, the Mott insulator is antiferromagnetic, whereas it becomes spin-rotating antiferromagnetic if $0 < \lambda / t < 1$ and spin-rotating ferromagnetic if $\lambda / t > 1$.

In figures 6(a)–(c), we plot the momentum distribution functions $n_i (k)$ and the gap $\Delta$ for the different filling factors $n$, when $\lambda / t = 1$ and $U/t = 10.0$. If $n \neq 1$, all sharp edges (Fermi points) in the momentum distribution functions $n_i (k)$ still exist and the zero gap, $\Delta \equiv 0$ (thermodynamical limit), remains, which indicates that the system is always located at the SOC-induced metallic phase for any on-site repulsive interaction strength $U/t$. However, at the half filling ($n = 1$), the momentum distribution function $n_i (k)$ becomes smoother and $\Delta = 0$ (thermodynamical limit) for any on-site repulsive interaction strength $U/t$, which mean these Mott insulators only occur at the half filling ($n = 1$), similar to the result without SOC [45].

### 4.2. Spin-correlation function and spin-structure factor

In figures 7(a)–(d), we plot the spin-correlation functions $s(r)$ for the different SOC strengths $\lambda / t$. These figures show clearly that in the presence of the on-site repulsive interaction ($U/t = 0$), quasi-long-range spin correlation appears, i.e., $s(r > 1) \neq 0$, which is in contrast to the result without the on-site repulsive interaction in which only the short-range spin correlation emerges (see figures 4(a) and (b)). When increasing the SOC strength $\lambda / t$, the spin-correlation functions between the nearest-neighbor sites vary from the negative to the positive. In order to see this physics more clearly, we plot, in figures 8(a)–(d), the spin distributions of each site, i.e., $s_i = \langle s_i^x, s_i^y, s_i^z \rangle$, where $s_i^x = \langle G | c_i^\dagger c_i | G \rangle$, $s_i^y = \langle G | c_i^\dagger c_i | G \rangle$, and $s_i^z = \langle G | c_i^\dagger c_i | G \rangle$ with the ground-state wavefunction $| G \rangle$, for the different SOC strengths $\lambda / t$. We define an intersection angle $\theta$ between the different spin orientations of the nearest-neighbor sites.

In the absence of SOC ($\lambda / t = 0$), the spin orientations of the nearest-neighbor sites are antiparallel and $\theta = \pi$ (see figure 8(a)). Moreover, the spin-correlation function $s(r) > 0$ if $r$ is odd, while $s(r) < 0$ if $r$ is even (see figure 7(a)). These mean the corresponding spin-spin interactions of the nearest-neighbor sites are antiferromagnetic. In addition, the spin-correlation function $s(r)$ decays as a power law and changes the sign with a period $T = 2$ [18] (see also figure 7(a)). This phase is usually called the antiferromagnetic Mott insulator. In the presence of SOC (see, e.g., $\lambda / t = 0.1$), the spin orientations of the nearest-neighbor sites are not
antiparallel (i.e., the spins are rotating) and $\pi/2 < \theta < \pi$ (see figure 8(b)). Since in this case the traditional spin-independent hopping still plays a dominate role, the quasi-long-range antiferromagnetic spin correlation remains, but with a period $2 < T < 4$ (see figure 7(b)). Thus, we call the corresponding phase the spin-rotating antiferromagnetic Mott insulator. When $\lambda/t = 1$, the spin orientations of the nearest-neighbor sites are vertical and $\theta = \pi/2$ (see figure 8(c)). Moreover, $s(1) = s(3) = \cdots = 0$ with a period $T = 4$, which means no spin correlation between the nearest-neighbor sites can be found (see figure 7(c)). At the strong SOC ($\lambda/t > 1$), the SOC-induced hopping plays a dominate role. In this case, the spin orientations of the nearest-neighbor sites tend to parallel and $\theta < \pi/2$ (see figure 8(d)). Moreover, $s(1) > 0$, which indicates the spin-spin interactions of the nearest-neighbors sites become ferromagnetic. In addition, the quasi-long-range spin-correlation function $s(r)$ also decays as a power law, but changes the sign with a period $T > 4$ (see figure 7(d)). We call the corresponding phase the spin-rotating ferromagnetic Mott insulator. From the above discussions, we argue that SOC can drive
the system from the spin-rotating antiferromagnetic Mott insulator to the spin-rotating ferromagnetic Mott insulator.

Figure 9(a) shows the experimentally-measurable spin-structure factors $S(k)$ for the different SOC strengths $\lambda/t$ at the half filling ($n = 1$). In the absence of SOC ($\lambda/t = 0$), the system has the antiferromagnetic order \[78, 87\], and the spin-structure factor $S(k)$ has a peak at the momentum $k_{\text{peak}} = \pi$, as expected. When increasing the SOC strength $\lambda/t$, the peak still exists and varies as $k_{\text{peak}} = 2k_{\text{max}} - \pi = 4 \arctan \left( \frac{t + \sqrt{t^2 + \lambda^2}}{\lambda} \right) - \pi$.\[15\]

It is easy to see from equation (15) that when $\lambda/t = 1$, $k_{\text{peak}} = \pi/2$ (see figure 9(b)). When $0 < \lambda/t < 1$, the system has the spin-rotating antiferromagnetic Mott insulator with $\pi/2 < k_{\text{peak}} < \pi$. When $1 < \lambda/t < 2$, the system has the spin-rotating ferromagnetic Mott insulator with $k_{\text{peak}} < \pi/2$. Since the antiferromagnetic order has been detected experimentally by measuring $k_{\text{peak}}$ via the time-of-flight imaging \[74\], these spin-rotating ferromagnetic and antiferromagnetic orders can also be detected by the same method. For a fixed SOC strength $\lambda/t = 1$, when increasing the on-site repulsive interaction strength $U/t$, the momentum $k_{\text{peak}}$ remains unchanged, while the magnitudes of peaks increase (see figure 9(c)). In figure 9(d), we present a finite-size-scaling analysis of the momentum $k_{\text{peak}}$ which figure shows that the momentum $k_{\text{peak}}$ remains unchanged when increasing the lattice length $L$.

### 4.3. Phase diagram

Based on the predicted properties of the momentum distribution, gap, and spin correlation, we find that the homogeneous Hamiltonian (3) has five phases, including the metallic phase, the SOC-induced metallic phase, the antiferromagnetic Mott insulator the spin-rotating antiferromagnetic Mott insulator, and the spin-rotating ferromagnetic Mott insulator at the half filling ($n = 1$). In the metallic phase, the system has conventional momentum distribution with the gap $\Delta \equiv 0$ (thermodynamical limit), while it becomes filling-dependent unconventional momentum distribution but with the same zero gap (thermodynamical limit) in the SOC-
induced metallic phase. In the antiferromagnetic, spin-rotating antiferromagnetic, and spin-rotating ferromagnetic Mott insulators, the system has a nonzero gap (thermodynamical limit) and the quasi-long-range spin correlation decays as a power law. However, in the antiferromagnetic Mott insulator, \( \theta = \pi \), \( T = 2 \), and \( k_{\text{peak}} = \pi \). In the spin-rotating antiferromagnetic Mott insulator, \( \pi / 2 < \theta < \pi \), \( 2 < T < 4 \), and \( \pi / 2 < k_{\text{peak}} < \pi \), whereas in the spin-rotating ferromagnetic Mott insulator, \( \theta < \pi / 2 \), \( T > 4 \), and \( k_{\text{peak}} < \pi / 2 \).

In figure 10, we show a schematic phase diagram as a function of the SOC strength \( \lambda / t \) and the on-site repulsive interaction strength \( U / t \). In this figure, the Mott insulator and the metallic phase are separated by the gap \( \Delta \) (thermodynamical limit) [45]. The metallic phase and the SOC-induced metallic phase are separated by the momentum distribution function \( n_{\uparrow}(k) \). The antiferromagnetic Mott insulator and the spin-rotating antiferromagnetic Mott insulator are separated by \( \theta = \pi \), \( T = 2 \), and \( k_{\text{peak}} = \pi \). The spin-rotating antiferromagnetic Mott insulator and the spin-rotating ferromagnetic Mott insulator are separated by \( \theta = \pi / 2 \), \( T = 4 \), and \( k_{\text{peak}} = \pi / 2 \).

We also find that the transitions between the metallic phase and the antiferromagnetic Mott insulator, between the SOC-induced metallic phase and the spin-rotating antiferromagnetic Mott insulator, and between the SOC-induced metallic phase and the spin-rotating ferromagnetic Mott insulator are of second order, because the second-order derivative of the ground-state energy is discontinuous at the critical points. For the other transitions, the ground-state energy and its derivative vary smoothly, which means, where no phase transition can be found, although for the different phases, the momentum distribution and the spin correlation are different.

5. Discussions and conclusions

Before ending up this paper, we make one remark. In the real experiment, the Zeeman field usually exists. When the Zeeman field is considered, an extra Hamiltonian should be added in the Hamiltonian (3). This Zeeman field can lead to spin flipping in the same site. Moreover, it has strong competition with SOC, which makes Fermi atoms hop between the nearest-neighbor sites with spin flipping and the conventional spin-independent hopping between the nearest-neighbor sites. As a consequence, rich magnetic properties can emerge. The deep understanding of relevant behavior is very complicated (we need to introduce more physical quantities), but interesting. We leave this important problem for future investigation.

In summary, we have investigated spin–orbit coupled repulsive Fermi atoms in a 1D optical lattice by the DMRG method. We found that SOC can generate the filling-dependent unconventional momentum distribution, whose corresponding phase is called the SOC-induced metallic phase, and drive the system from the spin-rotating antiferromagnetic Mott insulator to the spin-rotating ferromagnetic Mott insulator. We predicted a second-order quantum phase transition between the spin-rotating ferromagnetic Mott insulator and...
the SOC-induced metallic phase at the strong SOC. Finally, we showed that the momentum, at which peak of the spin-structure factor appears, can be affected dramatically by SOC. The analytical expression of this moment with respect to the SOC strength has also been derived. Attributed to the recent experimental realization of the spin–orbit coupled Bose–Einstein condensates in the 1D optical lattice [69], we expect that our predictions could be observed in the near future. In particular, the spin–rotating ferromagnetic and antiferromagnetic correlations can be detected by measuring the SOC-dependent spin-structure factor via the time-of-flight imaging [74].

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