Phase diagram, band structure and density of states in two-dimensional attractive Fermi-Hubbard model with Rashba spin-orbit coupling

Rui Han, Feng Yuan and Huaisong Zhao

College of Physics, Qingdao University, Qingdao 266071, People’s Republic of China

* Author to whom any correspondence should be addressed.

E-mail: hszhao@qdu.edu.cn

Keywords: ultracold atoms, optical lattice, Rashba spin–orbit coupling, topological superfluid, phase diagram

Abstract

Based on the two-dimensional (2D) attractive Fermi-Hubbard model with Rashba spin–orbit coupling (SOC), the SOC strength and Zeeman field dependences of the phase diagram are investigated by calculating the pairing gap self-consistently. The results reveal that the phase transition from the BCS superfluid to the topological superfluid happens under proper Zeeman field strength and SOC strength. In particular, in contrast to the BCS superfluid decreasing monotonically as the SOC strength increasing, the topological superfluid region shows a dome with the SOC strength increasing. An optimal region in the phase diagram to find the topological superfluid can be found, which is important to realize the topological superfluid in optical lattice experimentally. Then we obtain the change of both band structure and density of states (DOSs) during the topological phase transition, and explain the four peaks of DOS in the topological superfluid by the topology change of the low-energy branch of quasiparticle energy spectra. Moreover, the topological superfluid can be suppressed by the doping concentration.

1. Introduction

Rashba spin–orbit coupling (SOC) is closely related to many non-trivial physical properties [1–7], in particular for the topological superfluid state [8–12]. The topological superfluid state in the ultracold Fermi atomic system had been proposed by the coexistence of Rashba SOC, an external Zeeman field and s-wave pair order [13]. However, the Rashba SOC has not yet been realized experimentally until now. In recent years, by engineering the atom-laser interaction, the synthetic magnetic field, synthetic electric field and synthetic low-dimensional Raman-type SOC in the ultracold atomic system can be realized [14–27]. For the Raman-type SOC system, theoretically the topological superfluid will appear in one-dimensional (1D) Fermi atomic system, but it does not exist in two-dimensional (2D) Raman-type case. Degenerate 40K Fermi gases with 2D Raman-type SOC had been realized with a perpendicular Zeeman field [22] or an in-plane Zeeman field [25], respectively. To find the topological superfluid, we focus on how to realize the Rashba SOC in 2D ultracold atoms. Since the experimental breakthroughs in realization of Raman-type SOC in ultracold atomic gases, the region of topological superfluid state in phase diagram receives significant attention, which plays an important role in finding the topological superfluid state in experiments. Theoretically the phase diagrams were investigated in 2D polarized Fermi gas with Rashba SOC [8, 10, 28–31]. J Zhou and coworkers systematically studied the phase separation and gave the optimal parameter region for the preparation of the topologically nontrivial superfluid phase across a BCS (Bardeen-Cooper-Schrieffer)-BEC (Bose-Einstein condensate) crossover [8].

The periodic optical lattice potential confining cold atoms can be generated by superimposing orthogonal standing waves [32]. Experimentally the attractive Fermi-Hubbard model in cold atom systems had been realized [33–35], and the quantum phase transitions were discussed well [36–40]. In particular, the
optical lattice with the Rashba SOC is a good platform to study the topological phase transition [41–52]. By considering an in-plane Zeeman field in Fermi-Hubbard model, mean-field phase diagrams of 2D square optical lattice with Rashba SOC were given [41], and both Fulde–Ferrell and Larkin-Ovchinnikov phases may be observed [53–56]. A semimetal-superfluid transition in an optical lattice with the on-site attraction was induced by the SOC [43]. N. Goldman and coworkers found that when the system enters the non-Abelian gauge field regime, the two Van Hove singularities (VHS) in the density of states (DOSs) of an ultracold Fermi gas are split into four [46], which leads to that there are four peaks of the DOS in the non-Abelian gauge field regime. Based on a self-consistent mean-field theory in the optical lattice with the repulsive on-site interaction, L. Wang and coworkers discussed a quantum phase transition from a semimetallic phase to a band insulator and found the change of the energy spectra and DOS during the phase transition [49].

Although the Rashba-type SOC has not yet been realized experimentally, several theoretical proposals on how to realize it had been given [57–65]. And the optimal parameters to find the topological superfluid state in the Rashba SOC are still an open question. In this work, based on the mean-field theory of Fermi atom system, we study the phase transition from BCS superfluid to topological superfluid in 2D attractive Fermi-Hubbard model with synthetic Rashba SOC. Our results show that the optimal topological superfluid region exists when both the Zeeman field strength and Rashba SOC strength take appropriate values, i.e. the Zeeman field strength has a large adjustable range and the pairing gap is still large. Moreover, we discuss the effect of Rashba SOC interaction on the band structure and DOS during the phase transition from BCS superfluid to topological superfluid, then find the characteristic signals to distinguish two superfluid states. Although the quantum fluctuation of 2D system is large, the mean-field theory can still be expected to give a qualitatively reliable prediction.

Our paper is organized as follows. In the sections 2 and 3, we introduce the Green’s functions and the phase diagrams, respectively, then discuss the angle resolved photoemission spectroscopy (ARPES) and band structure in section 4. The SOC strength dependence of DOS is studied in section 5. Moreover, we discuss the doping dependent of phase diagrams in section 6, and give a summary in section 7.

2. Mean-field description with Green’s functions

It is widely believed that the attractive Fermi-Hubbard model captures the main physical properties of the Fermi superfluid in optical lattices. Therefore, it is important to study the attractive Fermi-Hubbard model with the SOC and Zeeman fields. For two-dimensional optical lattice with Rashba SOC and a perpendicular Zeeman field, the Hamiltonian can be described by the Fermi-Hubbard model,

\[
H = -t \sum_{\langle ij \rangle} C^\dagger_{i\sigma} C_{j\sigma} - U \sum_i C^\dagger_{i\uparrow} C_{i\downarrow} C_{i\downarrow} C^\dagger_{i\uparrow} - (\mu + \hbar \sigma_z) \sum_i C^\dagger_{i\sigma} C_{i\sigma} + \lambda \sum_i \left[ C^\dagger_{i+x\uparrow} C_{i\uparrow} - C^\dagger_{i+x\downarrow} C_{i\downarrow} + i(C^\dagger_{i+y\uparrow} C_{i\uparrow} + C^\dagger_{i+y\downarrow} C_{i\downarrow}) \right] + H.c.,
\]

where \(\langle ij \rangle\) means the nearest-neighbor sites of 2D lattice, \(\mu\) is the chemical potential, and \(U > 0\) is the on-site attraction strength. Parameters \(t, \lambda\) and \(\hbar\) are the strength of hopping, Rashba SOC and Zeeman field, respectively. \(C^\dagger_{i\sigma}(C_{i\sigma})\) is the atom creation (annihilation) operator with spin \(\sigma (\sigma = \uparrow, \downarrow)\) at the lattice \(i\). Here \(\sigma_z\) is the Pauli matrix. Within the mean field theory, the interaction part with the four operators can be dealt with \(U \sum_i C^\dagger_{i\uparrow} C_{i\downarrow} C_{i\downarrow} C^\dagger_{i\uparrow} = \sum_i (\Delta^* C_{i\uparrow} C_{i\downarrow} + \Delta C^*_{i\downarrow} C_{i\uparrow})\), where the pairing gap \(\Delta = U < C_{i\uparrow} C_{i\downarrow} >\).

Equation (1) has a simple BCS form within the mean-field theory in momentum space,

\[
H = \sum_{k,\sigma} \left( \varepsilon_k - \hbar \sigma_z \right) C^\dagger_{k\sigma} C_{k\sigma} + \sum_k [\lambda_{so}(k) C^\dagger_{k\uparrow} C_{k\downarrow} + \lambda_{so}^*(k) C^\dagger_{k\downarrow} C_{k\uparrow}] - \sum_k (\Delta^* C_{k\uparrow} C_{-k\downarrow} + \Delta C^*_{-k\downarrow} C_{k\uparrow}),
\]

where \(\varepsilon_k = -Z \gamma_1 \mu - \lambda_{so}(k) = \lambda(\sin k_x + i \sin k_y), \lambda_{so}^*(k) = \lambda(\sin k_x - i \sin k_y), \gamma_1 = 0.5(\cos k_x + \cos k_y)\), and the parameters \(Z = 4\) for 2D square lattice. The Hubbard energy \(U\) and lattice constant \(a_0 = 1\) can be used as the units of energy and length. In this study, \(t/U = 0.3\), temperature \(T/U = 0.001\). Then we define the diagonal Green’s function with spin up \(G_\uparrow(k, \tau - \tau') = -(TG_{k\uparrow}(\tau) C^\dagger_{k\downarrow}(\tau'))\). Then we define the off-diagonal Green’s function with pairing related terms \(G^\dagger(k, \tau - \tau') = -(TG^\dagger_{k\uparrow}(\tau) C^\dagger_{k\downarrow}(\tau'))\). The two SOC related terms, \(S(k, \tau - \tau') = -(TG_{k\downarrow}(\tau) C^\dagger_{k\uparrow}(\tau'))\). Based on the motion equation of Green’s function [66, 67], we can obtain these functions,
\[ G_1(k, \omega) = \sum_a \left[ \frac{U_{ak}^2}{\omega - E_{ak}} + \frac{V_{ak}^2}{\omega + E_{ak}} \right], \quad G_2(k, \omega) = \sum_a \left[ \frac{U_{ak}^2}{\omega - E_{ak}} + \frac{V_{ak}^2}{\omega + E_{ak}} \right], \]

\[ \Gamma(k, \omega) = \sum_a \left[ \frac{\alpha_{ak}}{\omega + E_{ak}} + \frac{\beta_{ak}}{\omega - E_{ak}} \right], \quad S(k, \omega) = \sum_a \left[ \frac{\lambda_{\alpha k}(k) E_{ak}}{\omega - E_{ak}} + \frac{\lambda_{\alpha k}^*(k) Q_{ak}}{\omega + E_{ak}} \right], \]

\[ F(k, \omega) = \sum_a \left[ \frac{\lambda_{\alpha k}(k) T_{ak}}{\omega - E_{ak}} + \lambda_{\alpha k}^*(k) W_{ak} \right], \]

where \( U_{ak}^2 = (\Omega_{ak}^+ + \Xi_{ak}^+)/\Sigma_{ak}, \quad V_{ak}^2 = (\Omega_{ak}^- - \Xi_{ak}^-)/\Sigma_{ak}, \quad U_{ak}^2 = (\Omega_{ak}+ \Xi_{ak})/\Sigma_{ak}, \quad V_{ak}^2 = (\Omega_{ak} - \Xi_{ak})/\Sigma_{ak}, \)

\[ \alpha_{ak} = \frac{E_{ak}^2 + 2h E_{ak} + h^2 - \xi_{a}^2 - \Delta^2 - \lambda_{\alpha}^2(k)}{\Sigma_{ak}}, \quad \beta_{ak} = -\frac{E_{ak}^2 - 2h E_{ak} + h^2 - \xi_{a}^2 - \Delta^2 - \lambda_{\alpha}^2(k)}{\Sigma_{ak}}, \]

\[ P_{ak} = \frac{E_{ak}^2 + 2h E_{ak} + \xi_{a}^2 - h^2 - \lambda_{\alpha}^2(k)}{\Sigma_{ak}}, \quad Q_{ak} = -\frac{E_{ak}^2 - 2h E_{ak} + \xi_{a}^2 - h^2 - \lambda_{\alpha}^2(k)}{\Sigma_{ak}}, \]

\[ T_{ak} = 2(h + \xi_{a})/\Sigma_{ak}, \quad W_{ak} = -T_{ak}, \quad \Omega_{ak} = 2(E_{ak} - E_{ak}^2)/E_{ak}, \quad \Omega_{ak}^2 = F_{ak}^2 - \frac{[(\xi_{a} + h)^2 + \Delta^2 + \lambda_{\alpha}^2(k)]E_{ak}}{\Sigma_{ak}}, \]

\[ \xi_{a} = (\xi_{a}^2 + h^2 - \lambda_{\alpha}^2(k))/\xi_{a}^2, \quad \Omega_{ak} = E_{ak}^2 - \frac{[(\xi_{a} + h)^2 + \Delta^2 + \lambda_{\alpha}^2(k)]E_{ak}}{\Sigma_{ak}}, \]

\[ \xi_{a} = (\xi_{a}^2 + \Delta^2)/\xi_{a}, \quad \Omega_{ak} = E_{ak}^2 - \frac{[(\xi_{a} + h)^2 + \Delta^2 + \lambda_{\alpha}^2(k)]E_{ak}}{\Sigma_{ak}}, \]

\[ E_{1k} = \sqrt{h^2 + \xi_{a}^2 + \Delta^2 + \lambda_{\alpha}^2(k) + 2\sqrt{h^2(\xi_{a}^2 + \Delta^2) + \xi_{a}^2 \lambda_{\alpha}^2(k)}}, \]

\[ E_{3k} = \sqrt{h^2 + \xi_{a}^2 + \Delta^2 + \lambda_{\alpha}^2(k) - 2\sqrt{h^2(\xi_{a}^2 + \Delta^2) + \xi_{a}^2 \lambda_{\alpha}^2(k)}}, \]

\[ n = \sum_{k,a} \left[ (U_{ak}^2 + E_{ak}^2) n_F(E_{ak}) + (V_{ak}^2 + E_{ak}^2) n_F(-E_{ak}) \right], \]

\[ 1 = \sum_{k,a} \left[ \frac{\alpha_{ak} - \beta_{ak}}{2 E_{ak}} n_F(E_{ak}) + \frac{\beta_{ak}}{2 E_{ak}} \right], \]

\[ E_{2\text{ext}} = 0 \]

\[ f(k_{M}) = (U_{1k}^2 + E_{1k}^2) n_F(E_{1k}) + (V_{1k}^2 + E_{1k}^2) n_F(-E_{1k}) + (\xi_{1k}^2 + \Delta^2 + h_{M}^2 + \lambda_{\alpha}^2(k_{M}))/E_{1k}, \]

\[ g(k_{M}) = (\alpha_{1k} - \beta_{1k}) n_F(E_{1k})/2 E_{1k} + \beta_{1k}/2 E_{1k} - h_{M}/E_{1k}, \]

3. Phase diagram in the \( h - \lambda \) plane at half-filling

As \( h \) increases, a transition from a nontopological BCS superfluid to a topological superfluid state appears at the critical Zeeman field strength \( h_{c1} \). Then stronger Zeeman field makes the superfluid disappear and the normal metal phase appears, i.e. \( \Delta = 0 \) at the superfluid transition point \( h_{c2} \), which can be solved simultaneously with the state of equation (5) to obtain \( \mu \) and \( h_{c2} \). What’s more, a metal–insulator transition appears at \( h_{c3} \) owing to the open of band gap which is the result of the Zeeman splitting. The phase diagrams in the \( h - \lambda \) plane for half-filling \( n = 1.0 \) are shown in figure 1. And \( h_{c1} \) (green solid line), \( h_{c2} \) (blue dashed line) and \( h_{c3} \) (red dotted line) mark the BCS-topological superfluid transition, superfluid-normal metal transition and normal metal–insulator transition, respectively.
Figure 1. (a) Phase diagram in the $h-\lambda$ plane of 2D optical lattice with Rashba SOC effect (BCS-SF, Topo-SF, normal metal phase and insulator phase); (b) pairing gap $\Delta$ as functions of $h$ and $\lambda$ for $t/U = 0.3, n = 1.0, T/U = 0.001$. And $h_c^1$ (green solid line), $h_c^2$ (blue dashed line) and $h_c^3$ (red dotted line) mark the BCS-topological superfluid transition, superfluid-normal metal transition and normal metal–insulator transition, respectively.

Figure 2. (a) Pairing gap $\Delta$ as a function of the Zeeman field strength $h$ for the Rashba SOC strength $\lambda/U = 0.1$ (black solid line), $\lambda/U = 0.3$ (green dashed line), $\lambda/U = 0.6$ (red long dashed line), and $\lambda/U = 0.9$ (blue dash-dotted line). (b) $\Delta$ vs $\lambda$ for $h/U = 0.15$ (black solid line), $h/U = 0.22$ (green dashed line), $h/U = 0.25$ (red long dashed line), and $h/U = 0.35$ (blue dash-dotted line) with $t/U = 0.3$. The topological phase transition points are marked by the circle symbols.

There are four distinct phase-separated regions in the phase diagram, namely, the BCS superfluid (BCS-SF), topological superfluid (Topo-SF), normal metal and insulator phases. With the increase of $\lambda$, the region of the BCS superfluid decreases monotonically and disappears at $\lambda/U = 1.31$. However, in contrast to the case of the BCS superfluid, the topological superfluid region between green solid line and blue dashed line shows a dome as a function of $\lambda$, i.e. it is proportional to $\lambda$ at the low $\lambda$ region, and reaches a maximum at the optimal $\lambda_{op}/U = 0.61$, then decreases when $\lambda > \lambda_{op}$. Therefore, to realize the topological superfluid of the Rashba SOC in optical lattice experimentally, it is necessary to select a reasonable $\lambda$ and $h$. In particular, the $\lambda$ has a optimal region $\lambda_{op}/U = 0.61$, where $h$ has a large adjustable range and the pairing gap is still large. The metal–insulator phase transition happens at $h_c^3/U = 1.2$, and related discussion had been given in 1D optical lattice with SOC [68]. In figure 1(b), we can find an interesting phenomenon, i.e. the pairing gap $\Delta$ as a function of $h$ in the low $\lambda$ region decreases precipitously around the topological transition point $h_c^1$ while it decreases gently with the increase of $h$ in the larger $\lambda$ region. Based on the different $h$-dependent behavior of parameters in different $\lambda$ region, first-order phase transition appears in the low $\lambda$ region and the second-order phase transition happens in the larger $\lambda$ region. Similar case had also been discussed in a trapped 2D polarized Fermi gas with Rashba SOC [8].

To show this more clearly, we have calculated the $h$ and $\lambda$ dependences of the pairing gap, and the results of $\Delta$ as a function of $h$ for the SOC strength $\lambda/U = 0.1$ (black solid line), $\lambda/U = 0.3$ (green dashed line), $\lambda/U = 0.6$ (red long dashed line), and $\lambda/U = 0.9$ (blue dash–dotted line) are plotted in figure 2(a). And $\Delta$ as a function $\lambda$ for $h/U = 0.15$ (black solid line), $h/U = 0.22$ (green dashed line), $h/U = 0.25$ (red long dashed line), and $h/U = 0.35$ (blue dash–dotted line) are shown in figure 2(b). It is shown clearly in figure 2(a), the
4. Band structure and ARPES

Phase transition is often accompanied by the change of excitation spectra which can be obtained by the angle-resolved photoemission spectroscopy (ARPES). In the Fermi atomic system, the ARPES has been used to investigate the single-particle excitations [35, 73, 74]. In particular, the single-particle excitations on different regions of the Brillouin zone can be measured experimentally by ARPES, which reflects the information of pairing gap (magnitude and symmetry), band structure and Fermi surface. The signal of ARPES is closely related to the spectral function \( A(k, \omega) \), \( I(k, \omega) = A(k, \omega) \rho(\omega) \). As functions of momentum and energy, the spectral function can shed light on the dispersion, then get the information of band structure. Theoretically the spectral function can be obtained by the imaginary of diagonal Green’s function, \( A(k, \omega) = -2\text{Im}G(k, \omega) \). In this paper, the spectral function of 2D optical lattice with Rashba SOC is expressed as \( A(k, \omega) = -\text{Im}[G_1(k, \omega) + G_2(k, \omega)] \). By using equation (3), then the spectral function has a form as,

\[
A(k, \omega) = \pi \sum_n [(U_{\alpha k}^2 + U_{\beta k}^2)\delta(\omega - E_{\alpha k}) + (V_{\alpha k}^2 + V_{\beta k}^2)\delta(\omega + E_{\alpha k})].
\]  

(7)

A sum rule is obtained by integrating over all frequencies, \( \int_{-\infty}^{\infty} A(k, \omega)d\omega \).

In figure 3, the dispersion along the high symmetry directions in the Brillouin zone by calculating \( A(k, \omega) = -2\text{Im}G(k, \omega) \) are mapped for the Zeeman field strength (a) \( h/U = 0.1 \) (BCS-SF), (b) \( h/U = 0.2 \) (BCS-SF), (c) \( h_{1T}/U = 0.211 \) (topological transition point), and (d) \( h/U = 0.22 \) (Topo-SF) with parameter \( \lambda/U = 0.15 \) and \( \lambda/U = 0.22 \). It is clearly shown that the energy spectra have four branches: \( E_{1k}, E_{2k}, -E_{3k}, \) and \( -E_{4k} \). The band gap decreases as \( h \) increases, then it has a simple form by using the equation (3), then the spectral function has a form as,

\[
A(k, \omega) = \pi \sum_n [(U_{\alpha k}^2 + U_{\beta k}^2)\delta(\omega - E_{\alpha k}) + (V_{\alpha k}^2 + V_{\beta k}^2)\delta(\omega + E_{\alpha k})].
\]  

5. DOSs

Now we discuss DOSs during the topological phase transition. The density states can be obtained by spectral function, \( \rho(\omega) = 1/2\pi \sum_k A(k, \omega) \), then it has a simple form by using the equation (7),

\[
\rho(\omega) = \frac{1}{2} \sum_{k\alpha} [(U_{\alpha k}^2 + U_{\beta k}^2)\delta(\omega - E_{\alpha k}) + (V_{\alpha k}^2 + V_{\beta k}^2)\delta(\omega + E_{\alpha k})].
\]  

(8)

We calculate the energy dependence of \( \rho(\omega) \) under different \( h \). We choose six typical Zeeman strength parameters, (a) \( h/U = 0.1 \) (BCS-SF), (b) \( h/U = 0.2 \) (BCS-SF), (c) \( h_{1T}/U = 0.211 \) (topological transition point), and (d) \( h/U = 0.22 \) (Topo-SF) with parameter \( \lambda/U = 0.15 \) and \( \lambda/U = 0.22 \). It is clearly shown that the energy spectra have four branches: \( E_{1k}, E_{2k}, -E_{3k}, \) and \( -E_{4k} \). The band gap decreases as \( h \) increases, then it has a simple form by using the equation (3), then the spectral function has a form as,

\[
A(k, \omega) = \pi \sum_n [(U_{\alpha k}^2 + U_{\beta k}^2)\delta(\omega - E_{\alpha k}) + (V_{\alpha k}^2 + V_{\beta k}^2)\delta(\omega + E_{\alpha k})].
\]  

(7)
Figure 3. Dispersion along the high symmetry directions for the Zeeman field strength (a) $h/U = 0.1$ (BCS-SF), (b) $h/U = 0.2$ (BCS-SF), (c) $h_{c1}/U = 0.211$ (topological transition point), and (d) $h/U = 0.22$ (Topo-SF) with parameter $\lambda/U = 0.15$.

It is shown that the DOS is strongly dependent on $h$, and is symmetric between positive and negative energy. Due to the modulation of SOC on the DOS, the DOS is affected not only by the pairing gap, but also by the strength of SOC. At the BCS superfluid, the weight of DOS disappears at the Fermi energy ($\omega = 0$) and locates at the high-binding energy region. With the increase of $h$, the weight of DOS moves towards the Fermi energy, and shows a sharp peak at the Fermi energy when $h = h_{c1}$, in which the excitation gap of $E_{2k_M}$ closes at $k_M$, ($E_{2k_M} = 0$). When $h > h_{c1}$, the weight of DOS moves back to the high-binding energy from the Fermi energy as the excitation gap reopens in the topological superfluid. Moreover, stronger $h$ in figure 5(e) will destroy the superfluid (then $\Delta = 0$) and the normal metal phase appears, thus the weight of DOS at the Fermi energy appears. When $h$ is over $h_{c3}$, the system will enter the insulator phase, in which the weight of DOS at the Fermi energy disappears as a result of the band gap. In particular, when the system enters the topological superfluid from the BCS superfluid, an interesting phenomenon about DOS can be found, i.e. there are three characteristic peaks in $h/U = 0.2$ (BCS-SF) while four characteristic peaks appear in $h/U = 0.22$ (Topo-SF). The characteristic peaks are marked by the arrows with a number. The abrupt change of characteristic peaks in DOS during the topological phase transition indicates the change of VHS which is associated with the quasiparticle energy spectra, $\rho(\omega) \propto (\nabla_k E_{2k})^{-1}$. Therefore, to study this problem clearly, we discuss the quasiparticle energy spectra from the BCS superfluid to the topological superfluid in the Brillouin zone.

Now we plot $E_{1k}$ (top row) and $E_{2k}$ (bottom row) for (a) (d) $h/U = 0.1$, (b) (e) $h_{c1}/U = 0.211$, (c) (f) $h/U = 0.22$ in figure 6. Our results show that with the increase of $h$, the low-energy quasiparticle spectrum $E_{2k}$ changes obviously from the BCS superfluid to the topological superfluid. On the one hand, around $k_M = [\pi, 0]$ marked by the red arrow, an excitation gap opens in both the BCS superfluid and the topological superfluid, and it vanishes at the topological phase transition point in figure 6(e) indicating the appearance of the gapless excitations. On the other hand, along the high symmetry direction $[0, 0] \rightarrow [\pi, 0] \rightarrow [2\pi, 0]$, the
Figure 4. Spectral function $A(k, \omega)$ as a function of $\omega$ at $k = k_M$ for (a) $h/U = 0.1$ (BCS-SF), (b) $h/U = 0.2$ (BCS-SF), (c) $h_{c1}/U = 0.211$ (topological transition point), and (d) $h/U = 0.22$ (Topo-SF), respectively.

Figure 5. Density of states as a function of $\omega$ for (a) $h/U = 0.1$ (BCS-SF), (b) $h/U = 0.2$ (BCS-SF), (c) $h_{c1}/U = 0.211$ (topological transition point), (d) $h/U = 0.22$ (Topo-SF), (e) $h/U = 0.6$ (normal metal), and (f) $h/U = 1.3$ (insulator) with $\lambda/U = 0.15$.

The lowest point of $E_{2k}$ is located at $k_M$ marked by the red arrow in the BCS superfluid, while in the topological superfluid state, it is located at position marked by the green arrow. To see these points clearly, the momentum dependence of $E_{1k}$ and $E_{2k}$ was calculated along $[0, 0] \rightarrow [\pi, 0] \rightarrow [2\pi, 0]$ in the Brillouin zone. The related results obtained for (a) $E_{1k}$ and (b) $E_{2k}$ as a function of momentum at $\lambda/U = 0.15$ for $h/U = 0.1$ (green dotted line), $h_{c1}/U = 0.211$ (red solid line), and $h/U = 0.22$ (blue dashed line) are plotted in figure 7. In the BCS superfluid with a small $h$, the lowest point for both $E_{1k}$ and $E_{2k}$ appears at $k_M$. When $h = h_{c1}$, $E_{2k}$ has a gapless excitation at $k_M$ and a linear Dirac-type dispersion appears. Going on increasing of $h$, the topological superfluid appears, in which the lowest point of $E_{2k}$ shifts from $\pi$ to a smaller momentum. Therefore, the topology of the quasi-particle energy spectrum $E_{2k}$ has a dramatic change during the topological phase transition from the BCS superfluid to the topological superfluid. Obviously, there are more momentum points satisfying $\nabla_k E_{2k} = 0$ in the topological superfluid. From $\rho(\omega) \propto (\nabla_k E_{2k})^{-1}$ as
Figure 6. Quasiparticle energy spectra $E_1$ (top row) and $E_2$ (bottom row) for (a) (d) $h/U = 0.1$, (b) (e) $h_1/U = 0.211$, (c) (f) $h/U = 0.22$ from the BCS superfluid to the topological superfluid in the full Brillouin zone.

Figure 7. Quasiparticle energy spectra (a) $E_1$ and (b) $E_2$ along the high symmetry direction $[0,0] \rightarrow [\pi,0] \rightarrow [2\pi,0]$ for $h/U = 0.1$ (green dotted line), $h_1/U = 0.211$ (red solid line), and $h/U = 0.22$ (blue dashed line) with $\lambda/U = 0.15$.

mentioned above, the DOS of the topological superfluid will have more peak. Moreover, the topology of the low-energy quasiparticle energy spectrum in 1D SOC Fermi gas has a similar change with increase of the Zeeman field [75].

Moreover, from the viewpoint of the topology of the low-energy quasiparticle energy spectrum, we try to discuss the change from the first-order (low $\lambda$) phase transition to the second-order (larger $\lambda$) phase transition with the increase of $\lambda$ as mentioned in figure 2. Along $[0,0] \rightarrow [\pi,0] \rightarrow [2\pi,0]$ in the Brillouin zone, we plot $E_2$ at (a) $h/U = 0.18$ (BCS-SF) and (b) $h/U = 0.225$ (Topo-SF) for the SOC strength $\lambda/U = 0.12$ (black solid line), $\lambda/U = 0.15$ (red dashed line), $\lambda/U = 0.27$ (green dotted line) and $\lambda/U = 0.35$ (blue dash-dotted line) in figure 8. It is shown that the topology of $E_2$ in both the BCS superfluid and topological superfluid is strongly dependent on the SOC strength. First, when $\lambda = 0$ and $h > 0$ (without SOC), a like traditional BCS state of superconductor will keep un-magnetized until a critical Zeeman field. Then a first-order phase transition appears from the BCS superfluid to the unpaired magnetized metal state [30]. Second, for the BCS superfluid, as $\lambda$ increasing, a kink structure around the green arrow appear. Third, for the topological superfluid, $E_2$ around $[\pi,0]$ (marked by the red arrow) is flat in the low $\lambda$ region and it decreases as $\lambda$ increasing. These results indicate that the symmetry of $E_2$ both the BCS superfluid and topological superfluid is changed with the increase of $\lambda$. We find that the symmetry change of energy spectra is accompanied by the change from first-order phase transition to second-order phase transition. In a word, the phase transition from the first-order to the second-order phase transition with the increase of $\lambda$ may be related to the symmetry change of energy spectra.
6. Doping dependence of phase diagram

For the Fermi system, the average occupancy number \( n = 1 - \delta \), where \( \delta \) is the doping concentration, and it indicates how far away the system is from half-filling. Doping can change the concentration of carrier, then greatly influence phase diagram and related physical properties. Now, we will discuss the phase diagram of 2D Rashba SOC lattice system when the system is away from half-filling. In figure 9, we plot the phase diagram in the \( h - \lambda \) plane for different average occupancy numbers: (a) \( n = 0.9 \) and (b) \( n = 0.8 \) at \( t/U = 0.3 \). The calculated results reveal that the phase diagram is strongly dependent on doping. As \( n \) decreases from half-filling, the topological superfluid region has shrunk while the region of BCS superfluid enlarges. Therefore, it is harder to realize the topological superfluid when the system is away from half-filling. Moreover, the insulator region disappears, which can be explained by the change of the quasiparticle energy spectra relative to the Fermi energy as \( n \) decreases: the low-energy quasiparticle energy spectrum always pass through the Fermi energy when the doping concentration exceeds a small amount. This phenomenon had been discussed in 1D optical lattice with Raman SOC \[68\].

7. Summary

The phase diagram, band structure and DOSs of Fermi atomic system in 2D optical lattice with Rashba SOC are discussed within the mean-field theory. The phase diagram in the \( h - \lambda \) plane shows that the topological superfluid appears under proper Zeeman field strength and SOC strength, and has an optimal Rashba SOC strength where the topological superfluid exists in a wide range of Zeeman field and the pairing gap is still large. Moreover, by calculating the spectral function, we obtain the change of both band structure and DOS
during the phase transition from BCS superfluid to topological superfluid. At the topological phase transition point, a Dirac dispersion appears in the low-energy quasiparticle energy spectrum, which leads to a sharp peak in the DOS at the Fermi energy. In the topological superfluid, the characteristic peaks of the DOS are one more than that of the BCS superfluid, which can be attributed to the topology change of the low-energy quasiparticle energy spectrum during the topological phase transition.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Acknowledgments

We are grateful to fruitful discussions with Professor Peng Zou. This work was supported by the funds from the National Natural Science Foundation of China under Grant Nos. 11547034, 11804177.

ORCID iDs

Feng Yuan  
https://orcid.org/0000-0003-1654-1103

Huaisong Zhao  
https://orcid.org/0000-0001-8774-9169

References

[1] Zhai H 2015 Rep. Prog. Phys. 78 026201
[2] Vyasanakere J P and Shenoy V B 2011 Phys. Rev. B 83 094515
[3] Vyasanakere J P, Zhang S Z and Shenoy V B 2011 Phys. Rev. B 84 014512
[4] Hu L, Jiang L, Liu X-J and Pu H 2011 Phys. Rev. Lett. 107 195304
[5] He L Y and Huang X-G 2013 Ann. Phys. 337 163–207
[6] Vyasanakere J P and Shenoy V B 2012 Phys. Rev. A 86 053617
[7] Zhang S-S, Yu X-L, Ye J W and Liu W M 2013 Phys. Rev. A 87 063623
[8] Zhou J, Zhang W and Yi W 2011 Phys. Rev. A 84 063603
[9] Liao Y, Rittner A S C, Paprotta P, Li W, Partridge G B, Hulet R G, Baur S K and Mueller E J 2010 Nature 467 567
[10] Cao Y, Zou S-H, Liu X-J, Pu H and Hu H 2014 Phys. Rev. Lett. 113 115302
[11] Zhou L H, Cui X L and Yi W 2014 Phys. Rev. Lett. 112 195301
[12] Hu H and Liu X-J 2013 New J. Phys. 15 093037
[13] Alicea J 2012 Rep. Prog. Phys. 75 076001
[14] Lin Y-J, Compton R L, Jiménez-García K, Porto J V and Spielman I B 2009 Nature 462 628
[15] Lin Y-J, Compton R L, Jiménez-García K, Phillips W D, Porto J V and Spielman I B 2011 Nat. Phys. 7 531
[16] Lin Y-J, Jiménez-García K and Spielman I B 2011 Nature 471 83
[17] Galitski V and Spielman I B 2013 Nature 494 49–54
[18] Cheuk L W, Sommer A T, Hadzibabic Z, Yefsah T, Bave W S and Zwierlein M W 2012 Phys. Rev. Lett. 109 095302
[19] Wang P, Yu Z-Q, Fu Z, Miao J, Huang L, Chai S, Zhai H and Zhang J 2012 Phys. Rev. Lett. 109 095301
[20] Zhang J, Hu H, Liu X-J and Pu H 2014 Annual Review of Cold Atoms and Molecules vol 2 (Singapore: World Scientific) pp 81–143
[21] Williams R A, Beeler M C, LeBlanc L C, Jiménez-García K and Spielman I B 2013 Phys. Rev. A 111 093051
[22] Meng Z M, Huang L H, Peng P, Li D H, Chen L C, Xu Y, Zhang C W, Wang P J and Zhang J 2016 Phys. Rev. Lett. 117 235304
[23] Huang L H, Peng P, Li D H, Meng Z M, Chen L C, Qi C L, Wang P J, Zhang C W and Zhang J 2018 Phys. Rev. A 98 013615
[24] Burdick N Q, Tang Y J and Lev B L 2016 Phys. Rev. X 6 031022
[25] Huang L H, Meng Z M, Wang P J, Peng P, Zhang S-L, Chen L C, Li D H, Zhou Q and Zhang J 2016 Nat. Phys. 12 540
[26] Wu Z, Zhang L, Sun W, Xu X-T, Wang B Z, Ji S-C, Deng Y J, Chen S, Li S-J and Pan W J 2016 Science 354 6308
[27] Zhang S C, He C D, Huijse E, Ren Z J, Song B and Jo G-B 2018 Sci. Rep. 8 18005
[28] Yang X S and Wan S L 2012 Phys. Rev. A 85 023633
[29] Liu X-J, Jiang L, Pu H and Hu H 2012 Phys. Rev. A 85 021603(R)
[30] Sheehy D E and Radzihovsky L 2007 Ann. Phys. 322 1790
[31] Zhang W and Yi W 2013 Nat. Commun. 4 2771
[32] Bloch I, Dalibard J and Zwerger W 2008 Rev. Mod. Phys. 80 885
[33] Mitra D, Brown P T, Guardado-Sanchez E, Kondov S S, Devakul T, Huse D A, Schauß P and Bakr W S 2018 Nat. Phys. 14 173
[34] Hackermüller L, Schneider U, Moreo-Cardonier M, Kitagawa T, Best W, Will S, Demler E, Altman E, Bloch I and Paredes B 2010 Science 327 1621
[35] Brown P T, Guardado-Sanchez E, Spar B M, Huang E W, Devereaux T P and Bakr W S 2020 Nat. Phys. 16 26–31
[36] Scalettar R T, Loh E Y, Gubernatis J E, Moreo A, White S R, Scalapino D J, Sugar R L and Dagotto E 1989 Phys. Rev. Lett. 62 1989
[37] Moreo A and Scalapino D J 1991 Phys. Rev. Lett. 66 946
[38] Singer J M, Pedersen M H, Schneider T, Beck H and Matutis H-G 1996 Phys. Rev. B 54 1286
[39] Paiva T, dos Santos R, Scalettar R T and Denteene P J H 2004 Phys. Rev. B 69 184501
[40] Ho A E, Cazalilla M A and Giamarchi T 2009 Phys. Rev. A 79 033620
[41] Xu Y, Qi C L, Gong M and Zhang C W 2014 Phys. Rev. A 89 013607
[42] Koinov Z and Fahl S 2017 Phys. Rev. A 95 033634
[43] Sun Q, Zhu G B, Liu W-M and Ji A-C 2013 Phys. Rev. A 88 063637
[44] Minar J and Grémaud B 2013 Phys. Rev. B 88 235130
[45] Riera J A 2013 Phys. Rev. B 88 045102
[46] Goldman N, Kubasiak A, Bermudez A, Gaspard P, Lewenstein M and Martin-Delgado M A 2009 Phys. Rev. Lett. 103 035301
[47] Iskin M 2013 Phys. Rev. A 88 013631
[48] Burrello M, Fulga I C, Alba E, Lepori L and Trombettoni A 2013 Phys. Rev. A 88 053619
[49] Wang L and Fu L B 2013 Phys. Rev. A 87 053612
[50] Qu C L, Zheng Z, Gong M, Xu Y, Mao L, Zou X B, Guo G C and Zhang C W 2013 Nat. Commun. 4 2710
[51] Jia W, Huang Z-H, Wei X, Zhao Q and Liu X-J 2019 Phys. Rev. B 99 094520
[52] Wu Y-J, Luo X-W, Hou J and Zhang C 2021 Phys. Rev. A 103 013307
[53] Liu X-J, Hu H and Drummond P D 2007 Phys. Rev. A 76 043605
[54] Wu F, Guo G-C, Zhang W and Yi W 2013 Phys. Rev. Lett. 110 110401
[55] Liu X-J and Hu H 2013 Phys. Rev. A 88 023622
[56] Yuan N F Q and Fu L 2021 PNAS 118 e2019063118
[57] Wang B-Z, Lu Y-H, Sun W, Chen S, Deng Y J and Liu X-J 2018 Phys. Rev. A 97 011605(R)
[58] Juzeliūnas G, Ruseckas J and Dalibard J 2010 Phys. Rev. A 81 053403
[59] Campbell D L, Juzeliūnas G and Spielman I B 2011 Phys. Rev. A 84 025602
[60] Xu Z F and You L 2012 Phys. Rev. A 85 043605
[61] Xu Z F, You L and Ueda M 2013 Phys. Rev. A 87 063634
[62] Zhou X F, Luo X-W, Chen G, Jia S T and Zhang C W 2019 Phys. Rev. A 100 063630
[63] Sau J D, Sensarma R, Powell S, Spielman I B and Sarma S D 2011 Phys. Rev. B 83 140510(R)
[64] Anderson B M, Spielman I B and Juzeliūnas G 2013 Phys. Rev. Lett. 111 125301
[65] Dalibard J, Gerbier F, Juzeliūnas G and Öhberg P 2011 Rev. Mod. Phys. 83 1523–43
[66] Zhao H, Gao X, Liang W, Zou P and Yuan F 2020 New J. Phys. 22 093012
[67] Gao Z, He L, Zhao H, Peng S-G and Zou P 2023 Phys. Rev. A 107 013304
[68] Han R, Yuan F and Zhao H 2022 Europhys. Lett. 139 25001
[69] Lee J and Kim D H 2017 Phys. Rev. A 95 033609
[70] Hu H, Jiang L, Liu X-J and Pu H 2011 Phys. Rev. Lett. 107 195304
[71] He L Y and Huang X-G 2012 Phys. Rev. Lett. 108 145302
[72] Zhou X Z and Zhang Z D 2012 Phys. Rev. Lett. 108 025301
[73] Stewart J T, Gaebler J P and Jin D S 2008 Nature 454 744
[74] Feld M, Fröhlich B, Vogt E, Koschorreck M and Köhl M 2011 Nature 480 75
[75] Fan G, Chen X L and Zou P 2022 Front. Phys. 17 52502