Spin-orbit Coupling Effects on the Superfluidity of Fermi Gas in an Optical Lattice

Q. Sun, G.-B. Zhu, W.-M. Liu, and A.-C. Ji^{2,1,*}

¹Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China ²Department of Physics, Capital Normal University, Beijing 100048, China (Dated: August 20, 2018)

We investigate the superfluidity of attractive Fermi gas in a square optical lattice with spin-orbit coupling (SOC). We show that the system displays a variety of new filling-dependent features. At half filling, a quantum phase transition from a semimetal to a superfluid is found for large SOC. Close to half filling where the emerging Dirac cones governs the behaviors of the system, SOC tends to suppress the BCS superfluidity. Conversely, SOC can significantly enhance both the pairing gap and condensate fraction and lead to a new BCS-BEC crossover for small fillings. Moreover, we demonstrate that the superfluid fraction also exhibits many interesting phenomena compared with the spin-orbit coupled Fermi gas without lattice.

PACS numbers: 67.85.Lm, 03.75.Ss, 05.30.Fk, 37.10.Jk

The spin-orbit coupling (SOC) plays a central role in the investigation of novel topological states in solid state physics [1, 2]. This has stimulated tremendous interests in creating artificial non-Abelian gauge fields in ultracold atom systems [3]. The successful realization of SOC in both Bose-Einstein condensate (BEC) [4, 5] and Fermi gas [6, 7] opens up a new avenue towards studying the rich physics of spin-orbit (SO) coupled ultracold atoms [8–13]. One of the important advances is that SOC was shown to have fundamental effects on the superfluidity of 3D [14–19] and 2D [19, 20] continuous Fermi gases.

On the other hand, the attractive Fermi gas subjected to an optical lattice [21, 22] has made it possible to simulate the negative-U Hubbard model, a basic model for the superconductivity of many solid state materials [23]. In particular, the on-site attractions can induce deep bound states, which cause the conventional BCS-BEC crossover. Recently, SOC has been combined to optical lattices for repulsive ultracold gases and predicted to lead to many interesting phenomena [24-26]. Nevertheless, the superfluidity of SO coupled attractive Fermi gas in an optical lattice remains a new frontier to be explored.

In this Letter, we study the Fermi gas subjected to a square optical lattice with SOC. Such a system can be described by a generalized negative-U Hubbard model. We show that, the combination of SOC and lattice can give rise to various new features that depend on the fillings. Remarkably, there develops a quantum phase transition (QPT) from a semimetal to a superfluid for large SOC at half filling, with the critical interaction $U_c/t \simeq 3.11$ (t is the hopping amplitude). For close to half filling, we show that the emerging Dirac cones governs the behaviors of the system, which tends to suppress the BCS superfluidity. By contrary, SOC can significantly enhance both the pairing gap and condensate fraction and lead to a new BCS-BEC crossover for small fillings. Compared with the SO coupled Fermi gas without lattice, such opposite filling-dependent behavior of SOC is rather unique as it can only be induced in the lattice system. Furthermore,

we investigate the superfluid fraction, which also exhibits many unusual characteristics in contrast to the continuous Fermi gas.

We consider a system of two-component Fermi gas moving in an optical square lattice. In the tight binding approximation, the Hamiltonian reads

$$H = -t \sum_{\langle ij \rangle} \sum_{\sigma\sigma'} (c_{i\sigma}^{\dagger} R_{ij} c_{j\sigma'} + \text{H.c.})$$
$$-U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i} n_{i}, \qquad (1)$$

where t is the overall hopping amplitude and $c_{i\sigma}^{\dagger}$ is the creation operator for spin-up (down) fermion $\sigma = \uparrow, \downarrow$ at site i. The nearest sites tunneling matrices $R_{ij} = e^{i\vec{A}\cdot(\vec{r}_j-\vec{r}_i)}$ with $\vec{A} = \lambda\left(\sigma_x,\sigma_y\right)$ the non-Abelian gauge-field [24–27], λ is the strength of Rashba SOC [28] (see Fig. 1(a)). Here, the diagonal term of R_{ij} denotes the spin-conserved hopping, while the non-diagonal term can be realized by the Raman laser assisted spin-flipped tunneling [29]. U is the on-site attraction strength which can be tuned by Feshbach resonances and μ is the chemical potential. $n = \langle n_{i\uparrow} + n_{i\downarrow} \rangle$ is the filling factor.

Fig. 1(b) shows the band structure of non-interacting fermions, where SOC lifts the spin degeneracy and gives rise to two split Rashba bands. Remarkably, the two bands intersect linearly at $\Gamma = (0,0), M = (\pi,0), (0,\pi)$ and $K = (\pi, \pi)$. The zero energy Fermi surfaces at half filling is shown in Fig. 1(c), where we have a particle (hole) Fermi-pocket around Γ (K) which is associated to the up (down) Rashba band respectively. Note that, there always exist two zero energy Fermi points at Mfor any $\lambda \neq 0$. Specifically, when $\lambda = \pi/2$, both the particle (hole) Fermi-pockets shrink to Fermi points at zero energy, and there develops a semimetal with four Dirac cones at Γ , K and M. Fig. 1(d) shows the density of states (DOS) $\rho(E)$ of single-particle excitation over the regime $\lambda \in [0, \pi/2]$, we see that when $\lambda = \pi/2$, $\rho(E) \propto$ |E| which vanishes linearly around zero energy.

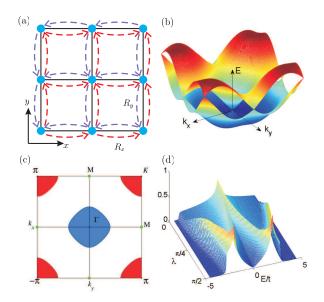


FIG. 1: (color online) (a) SO coupled square optical lattice, where $R_{x(y)}$ denotes the non-Abelian hopping matrice along x(y) direction. (b) Energy bands of non-interacting fermions with $\lambda=3\pi/10$ for illustration. (c) Zero energy Fermi surfaces at half filling, where the filled particle (blue) and hole (red) Fermi pockets represent the up/down Rashba band respectively. The green dots denote two zero energy Fermi points at M. (d) Density of states $\rho(E)$ over the regime $\lambda \in [0,\pi/2]$.

We start by writing the partition function in the imaginary-time path integral $\mathcal{Z}=\int \mathcal{D}[\bar{\psi},\psi]e^{-S[\bar{\psi},\psi]},$ where $S[\bar{\psi},\psi]=\int_0^\beta d\tau [\sum_\sigma \bar{\psi}_\sigma \partial_\tau \psi_\sigma + H(\bar{\psi},\psi)]$ with $\psi=(\psi_\uparrow,\psi_\downarrow)^T$ representing the Grassmann field variables. Then, by decoupling the attractive term of Eq. (1) in normal and anomalous channels through a pairing field $\Delta_i(\tau)=U\psi_{i\downarrow}(\tau)\psi_{i\uparrow}(\tau)$ and introducing $(\psi_{\mathbf{k}\uparrow},\psi_{\mathbf{k}\downarrow},\bar{\psi}_{-\mathbf{k}\uparrow},\bar{\psi}_{-\mathbf{k}\downarrow})^T$, we obtain the effective action after integrating out the fermionic field $S_{\mathrm{eff}}=\sum_i \int_0^\beta d\tau \frac{|\Delta_i(\tau)|^2}{U} - \frac{1}{2}\mathrm{Tr}\ln\mathcal{G}^{-1} + \beta\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}$. Here we have ignored the constant term $NUn^2/4$ (N is the number of lattice sites) and the inverse Green function is given by

$$\mathcal{G}^{-1} = \begin{pmatrix} \partial_{\tau} + \varepsilon_{\mathbf{k}} + \lambda_{\mathbf{k}} & -i\sigma_{y}\Delta_{i}(\tau) \\ i\sigma_{y}\bar{\Delta}_{i}(\tau) & \partial_{\tau} - \varepsilon_{\mathbf{k}} + \bar{\lambda}_{\mathbf{k}} \end{pmatrix}, \quad (2)$$

with $\varepsilon_{\mathbf{k}} = -2t \cos\lambda(\cos k_x + \cos k_y) - \bar{\mu}$ and $\lambda_{\mathbf{k}} = -2t \sin\lambda(\sin k_x \sigma_x + \sin k_y \sigma_y)$, where $\bar{\mu} = \mu + Un/2$ is the scaled chemical potential. Furthermore, we set $\Delta_i(\tau) = \Delta + \delta\Delta$ and write $\mathcal{G}^{-1} = \mathbf{G}^{-1} + \Sigma$ with $\mathbf{G}^{-1} = \mathcal{G}^{-1}|_{\Delta_i(\tau)=\Delta}$. Then, the effective action can be expanded to the second order of fluctuation Σ as $S_{\mathrm{eff}} \simeq S_0 + \Delta S$ with $S_0 = \frac{\beta N}{U} \sum |\Delta|^2 + \frac{1}{2} \sum_{\mathbf{k},\nu=\pm} \left[\frac{\beta}{2} (\varepsilon_{\mathbf{k}} - E_{\mathbf{k},\nu}) - \ln(1 + e^{-\beta E_{\mathbf{k},\nu}})\right]$, and $\Delta S \equiv \sum_q \Gamma^{-1}(q)\delta\bar{\Delta}(-q)\delta\Delta(q) = \frac{N}{U} \sum_q \delta\bar{\Delta}(-q)\delta\Delta(q) + \frac{1}{4}\mathrm{Tr}[G(k)\Sigma(-q)G(k-q)\Sigma(q)]$. Here $k = (\mathbf{k}, iw_n)$, $q = (\mathbf{q}, i\nu_n)$, and $E_{\mathbf{k},\pm} = \sqrt{\xi_{\mathbf{k},\pm}^2 + \Delta^2}$ with $\xi_{\mathbf{k},\pm} = \varepsilon_{\mathbf{k}} \pm 2t \sin\lambda \mathcal{K}$ being the two Rashba branches,

 $\mathcal{K} \equiv \sqrt{\sin^2 k_x + \sin^2 k_y}$. At the mean-field level, the many-body ground state of the system can be derived by minimizing $S_0/(N\beta)$ with respect to Δ and μ , and we have the following gap and Fermi density equations

$$\frac{1}{U} = \frac{1}{N} \sum_{\mathbf{k},\nu=\pm} \frac{1}{4E_{\mathbf{k},\nu}} \tanh(\frac{\beta E_{\mathbf{k},\nu}}{2}),$$

$$n = 1 - \frac{1}{N} \sum_{\mathbf{k},\nu=\pm} \frac{\varepsilon_{\mathbf{k}}}{2E_{\mathbf{k},\nu}} \tanh(\frac{\beta E_{\mathbf{k},\nu}}{2}). \tag{3}$$

Before proceeding, it's useful to consider the large attraction limit with $U/t \gg 1$. In this case, the standard degenerate perturbation theory can be applied for Eq. (1) through the canonical transformation $c_{i\uparrow} \rightarrow c_{i\uparrow}$ and $c_{i\downarrow} \to (-1)^{i_x+i_y} c_{i\downarrow}^{\dagger}$ [30]. For any band filling, we can derive an effective spin model $H_{\rm spin} = J \sum_{\langle ij \rangle} \mathbf{S}_i$. $\mathbf{S}_{i} - 2\bar{\mu} \sum_{i} S_{i}^{z}$ in the presence of arbitrary \overline{SOC} . Here $J = 4t^2/U$ and the pairing field operator becomes the transverse magnetic operator. For $\bar{\mu} \neq 0$, the antiferromagnetic order in XY plane is equivalent to the pairing order of Eq. (1). Therefore, we conclude that SOC does not have any influence on the superfluidity of the system in the large U limit, where all the fermionic atoms form tightly bound molecules and give rise to a Kosterlitz-Thouless transition of BEC [31]. In the following, we shall focus on the more interested weak and intermediate attraction regions.

The pairing gaps at zero temperature are illustrated in Fig. 2. First for half filling (n = 1), Fig. 2 (a) shows that the BCS gap decreases monotonically with respect to λ . This could be understood that, the Fermi pockets around Γ and K (see Fig. 1(c)) tend to form the Fermi points at $E_F = 0$ by increasing SOC, which causes a suppression of DOS at zero energy (see Fig. 1(d)). Specifically, when $\lambda = \pi/2$ the system becomes a semimetal, which is expected to be stable towards small attractions. On the other hand, when $U/t \gg 1$ the system should support a superfluid state of bound molecules as indicated by the effective spin model $H_{\rm spin}$ [32]. Hence, there must undergo a significant QPT from a semimetal to a superfluid by increasing attractions, see the thick vertical line of Fig. 2 (a). In the inset, we show that the critical value $U_c/t \simeq 3.11$, above which a finite gap develops.

Such scenario would be affected remarkably by dopings as shown in Fig. 2 (b). Without loss of generality, We focus on the hole doping case due to the particle-hole symmetry of the system. First for small dopings, similar to that of half filling, the superfluidity is governed by emerging Dirac cones at zero energy and Δ is suppressed by increasing λ , see n=0.95. However, when close to $\lambda=\pi/2$, the doping would make the QPT at half filling unstable and opens a gap. This produces a nonmonotonic behavior of Δ with a minimum at λ_{\min} . While for large dopings, the situation is entirely changed, where the influence of Dirac cones would diminish and SOC induces

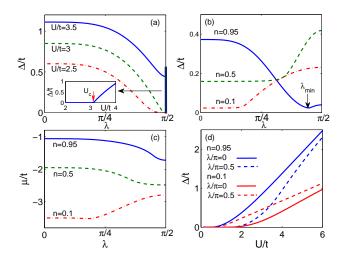


FIG. 2: (color online) (a) Plot of Δ versus λ at half filling for different U/t. Inset shows a semimetal-superfluid QPT with $U_c/t \simeq 3.11$. (b) Plot of Δ and (c) μ versus λ with U/t = 2 for different fillings. (d) Pairing gap as a function of U/t for two typical fillings with n = 0.1 (red) and 0.95 (blue). Solid and dashed lines represent $\lambda = 0$ and $\pi/2$ respectively.

a new BCS-BEC crossover with Δ being significantly enhanced, see the dash dotted line of n=0.1. This can be understood by solving the two-body problem of Eq. (1), which is determined by $\Gamma^{-1}(i\nu_n \to \omega + i0^+, \mathbf{q} = 0) = 0$ as $\omega + 2\bar{\mu} = -E_B$ and we arrive at

$$\frac{1}{U} = \frac{1}{2N} \sum_{\mathbf{k},\nu = +} \frac{1}{2(\xi_{\mathbf{k},\nu} - E_0) - E_B},\tag{4}$$

where E_0 denotes the lowest energy of $\xi_{\mathbf{k},-}$ branch. In the absence of SOC ($\lambda=0$), the binding energy $|E_B|/t\sim 0$ in the weak attraction region U/zt<1 (z=4 is the number of the nearest neighbor) and becomes very large for $U/zt\gg 1$, evolving from loosely local pairs (BCS) to tightly bound molecules (BEC) [23]. However, when SOC is added to the lattice, $|E_B|/t$ will be significantly enhanced (left panel of Fig. 3) due to the increasing of DOS around E_0 and effective shrinking of the bandwidth

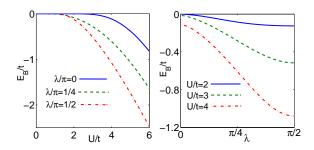


FIG. 3: (color online) Binding energy E_B/t as a function of U/t (left panel) and SOC strength λ (right panel).

(see Fig. 1(d)) [33]. In particular, the right panel shows

a remarkable grow of $|E_B|/t$ from nearly zero in the weak attraction regions, which signifies the formation of SOC induced bound states, see U/t = 2, 3 for example.

In general, such filling-dependent effects arise from the unique features of combination of SOC and lattice. The opposite behaviors of Δ versus SOC upon dopings indicate that the system evolves from the Dirac cone dominated physics near half filling to the SOC induced BCS-BEC crossover at small fillings. In this respect, the gap behavior at small fillings is reminiscent of SO enhanced pairing in the unitary Fermi gas [14–20]. However, we note that the lattice also plays nontrivial roles even in this limit. In Fig.2 (c), we see that μ increases with SOC at n=0.1, which differs from the familiar results in the continuous system where μ is decreased by SOC.

The opposite roles of SOC in lattice can be clearly seen in Fig. 2 (d), where we plot Δ as a function of U/t for two typical fillings. We take $\lambda = \pi/2$ for illustration and show that the strong SOC can remarkably enhance (n=0.1) or suppress (n=0.95) the pairing gaps of the conventional BCS-BEC crossover of negative-U Hubbard model, especially in the weak and intermediate attraction regions. While in the large attraction limit, Δ versus U/t approaches the $\lambda=0$ results, which means the SOC effects diminish according to the effective theory of $H_{\rm spin}$.

To get more insight of the unusual properties of this system, we now explore the condensate and superfluid fractions. First, the condensate density $n_c = \frac{1}{N} \sum_{\mathbf{k},\sigma,\sigma'} |\langle \psi_{\mathbf{k}\sigma} \psi_{-\mathbf{k}\sigma'} \rangle|^2$ [34], where the singlet and induced triplet pairing fields $\langle \psi_{\mathbf{k}\uparrow} \psi_{-\mathbf{k}\uparrow} \rangle = -\frac{\Delta}{4} e^{-i\theta_{\mathbf{k}}} \sum_{\nu} \frac{\nu}{E_{\mathbf{k},\nu}}$ and $\langle \psi_{\mathbf{k}\uparrow} \psi_{-\mathbf{k}\downarrow} \rangle = -\frac{\Delta}{4} \sum_{\nu} 1/E_{\mathbf{k},\nu}$ with $\theta_{\mathbf{k}} = \arg(\sin k_x + i \sin k_y)$. While for the superfluid density, we impose a phase twist on order parameter $\Delta \to \Delta e^{i\nabla\theta\cdot\vec{r}_j}$ by a local unitary transformation $\psi_j \to \psi_j e^{i\theta(\vec{r}_j)}$. Then, the inverse Green function can be written as $\mathbf{G}^{-1}[\Delta, \nabla\theta] = \mathbf{G}^{-1}[\Delta] + \Sigma[\nabla\theta]$. After lengthy but straightforward calculations, we derive a classical phase variation model $\widetilde{H} = \frac{1}{2}J\int d^2\mathbf{r}[(\partial_x\theta)^2 + (\partial_y\theta)^2]$ with J the phase stiffness. Therefore, the superfluid density can be defined as $\rho_s = \frac{J}{2tN}$, which reads

$$\rho_{s} = \frac{\cos\lambda}{N} \sum_{\mathbf{k}} \cos k_{x} n_{\mathbf{k}} + \frac{\sin\lambda}{N} \sum_{\mathbf{k},\nu} \frac{\nu \xi_{\mathbf{k},\nu}}{2E_{\mathbf{k},\nu}} \frac{\sin^{2}k_{x}}{\mathcal{K}} \tanh(\frac{\beta E_{\mathbf{k},\nu}}{2})$$

$$+ \frac{2t}{N} \sum_{\mathbf{k},\nu} f'(E_{\mathbf{k},\nu}) \sin^{2}k_{x} \left(\cos\lambda + \nu \frac{\sin\lambda\cos k_{x}}{\mathcal{K}}\right)^{2}$$

$$- \frac{\sin\lambda}{N} \sum_{\mathbf{k},\nu} \nu \frac{\varepsilon_{\mathbf{k}}^{2} + \nu 2t \sin\lambda \mathcal{K} \varepsilon_{\mathbf{k}} + \Delta^{2}}{2\varepsilon_{\mathbf{k}} E_{\mathbf{k},\nu}} \frac{\sin^{2}k_{y} \cos^{2}k_{x}}{\mathcal{K}^{3}}$$

$$\times \tanh(\frac{\beta E_{\mathbf{k},\nu}}{2}). \tag{5}$$

Here $n_{\mathbf{k}} = 1 - \sum_{\nu=\pm} \frac{\varepsilon_{\mathbf{k}}}{2E_{\mathbf{k},\nu}} \tanh(\frac{\beta E_{\mathbf{k},\nu}}{2})$ and the third term vanishes at T = 0. Not that, although the first and fourth terms bear similarities with the continuous

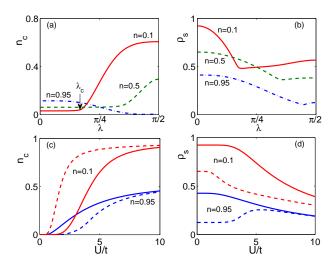


FIG. 4: (color online) (a) Condensate density n_c and (b) superfluid density ρ_s (both divided by n) at T=0 as a function of SOC for different fillings, where we take U/t=2. (c) Plot of n_c and (d) ρ_s versus U/t for two typical fillings with n=0.1 (red) and 0.95 (blue). Solid and dashed lines represent $\lambda=0$ and $\pi/2$ respectively.

system [19, 20], they may become negative in the lattice. Fortunately, the new second term which exists only in the SO coupled lattice system, can stabilize the superfluidity and gives rise to many intriguing features.

Fig. 4 (a) shows the condensate fraction n_c versus SOC with the evolution of fillings. For n=0.1, we see that n_c increase dramatically above a characteristic value λ_c , which agrees with the formation of the SOC induced bound states. The characteristic value λ_c grows with increasing fillings, and until $n \simeq 0.7$, n_c begins to decrease with respect to λ . This indicates that the BCS superfluidity would be suppressed at large fillings, see n=0.95 for example. On the contrary, the superfluid fraction ρ_s is always suppressed by SOC and generally decreased with increasing n, as shown in Fig. 4 (b). Significantly, there exhibits a characteristic minimum of λ , which moves rightwards when n is increased.

In Fig. 4 (c) and (d), we plot n_c and ρ_s with respect to U/t for two typical fillings. Qualitatively different from the conventional BCS-BEC crossover, the condensate fraction is remarkably enhanced (n=0.1) or suppressed (n=0.95) by the strong SOC. Conversely, the superfluid fraction is destroyed by both increasing U/t and λ . Intersetingly, ρ_s exhibits quite a nontrivial behavior at large fillings. The presence of strong SOC can dramatically suppress ρ_s for the weak attractions and causes a maximum of ρ_s located at the intermediate crossover region, see n=0.95 for example. While in the large attraction limit, both n_c and ρ_s will approach the results without SOC.

In summary, we have shown that the SO coupled Fermi gas in an optical lattice displays various new filling-

dependent features. At half filling, we find a QPT from a semimetal to a superfluid for large SOC. While upon dopings, the system evolves from the Dirac cone dominated physics near half filling to the SOC induced BCS-BEC crossover at small fillings. Moreover, we show that all the pairing gap, condensate and superfluid fractions exhibit many interesting physics, which differ qualitatively from the SO coupled Fermi gas without lattice and the conventional negative-U Hubbard model without SOC. We hope that this work will trigger new exciting interests to the SO coupled optical lattice physics, and may be useful for the study of superconductivity of future solid state materials with SOC.

We acknowledge Hui Zhai, G. Juzeliūnas, and X. F. Zhang for helpful discussions. We are grateful to Hui Zhai for reading the manuscript. This work is supported by NCET, NSFC under grants Nos. 11074175, 10934010, NSFB under grants No.1092009, NKBRSFC under grants Nos. 2011CB921502, 2012CB821305, and NSFC-RGC under grants No. 11061160490.

- * Electronic address: acji@iphy.ac.cn
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