Topological superfluid of spinless Fermi gases in $p$-band honeycomb optical lattices with on-site rotation

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Abstract – In this letter, we put forward another way for realizing topological superfluid (TS). In contrast to conventional method, spin-orbit coupling and external magnetic field are not requisite. Introducing an experimentally feasible technique called on-site rotation (OSR) into $p$-band honeycomb optical lattices for spinless Fermi gases and considering CDW and pairing on the same footing, we investigate the effects of OSR on superfluidity. The results suggest that when OSR is beyond a critical value, where CDW vanishes, the system transits from a normal superfluid (NS) with zero TKNN number to TS labeled by a non-zero TKNN number. In addition, phase transitions between different TSs are also possible.

Introduction. – Topological superfluid (or superconductor) (TS) has a full pairing gap in the bulk and is labeled by a non-zero integer topological invariant [1,2]. From the famous bulk-boundary correspondence such a topological integer ensures the existence of gapless excitations on the boundary of the system, in other words Majorana fermions (MFs) [3] in the vortex core of the pairing order parameter. Roughly, MFs are neither fermions nor bosons but non-Abelian anyons [4] and play an important role for the realization of fault-tolerant topological quantum computation (TQC) [5]. The application prospect of MFs makes TS become one of the hottest frontiers.

In the condensed-matter physics some practical two-dimensional systems have been theoretically proposed to realize TS [6–13]. In terms of these systems the entrance into TS requires subtle adjustment of Hamiltonian and it is very difficult in condensed-matter physics, although MFs have been detected in InSb nanowires contacted with one normal (Au) and one superconducting electrode (NbTiN) [14]. In the light of the disadvantage for condensed matter, TS has been also suggested in cold Fermi gases owing to their many controllable advantages and operabilities. Following the successful observation of the $p$-wave Feshbach resonance (FR), Guralie et al. [15] showed that degenerate Fermi gases near a $p$-wave FR naturally give a concrete realization of TS. Zhang et al. [16] proposed to create TS directly from an $s$-wave interaction making use of an artificially generated spin-orbit coupling (SOC). In fact, SOCs have been realized in a neutral atomic Bose-Einstein condensate (BEC) by dressing two atomic spin states with a pair of lasers and the same technique is also feasible for cold Fermi gases [17,18]. Realizing that in a dual transformation SOC is formally equivalent to a $p$-wave superfluid gap, Sato et al. [19] suggested to artificially generate the vortices of SOC by using lasers carrying orbital angular momentum. In terms of the latter two ways, SOC and a large magnetic field are crucial in order to enter into TS.

In this paper we suggest to create TS from spinless Fermi gases in $p$-band honeycomb optical lattices with the so-called on-site rotation (OSR), that rotates every lattice site around its own center but keeps the whole lattice intact and has been realized for triangular optical lattices [20]. As a matter of fact $p$-band Fermi gases in honeycomb optical lattices in the absence of OSR have shown many interesting characteristics, such as ferromagnetism [21] and Wigner crystallization [22,23] associated with flat bands, $f$-wave superfluidity with conventional pairing interaction [24]. The motivation for this paper comes from Wu’s work on the quantum anomalous Hall effect in the same system [25]. Under the single-particle picture, Wu found that an arbitrary non-zero OSR not
only breaks time-reversal symmetry and changes the topology of the system, but it also drives a topological phase transition when OSR is beyond a critical value. Here we add an on-site attraction interaction between $p$-band Fermi atoms into the Hamiltonian and ask whether OSR can drive a phase transition into TS. The results are positive and OSR brings phase transitions not only from normal superfluid (NS) to TS, but also among different TSs. From another perspective our work also can be considered as an extension to [24], where $f$-wave superfluidity without OSR is discussed. Thus, we also investigate the effects of OSR on $f$-wave superfluidity.

Experimentally the way to realize TS suggested here is also feasible. On the one hand, by placing two electro-optic modulators at two of three laser beams which coherently superpose to form a honeycomb lattice, OSR is available as illustrated in [26]. On the other hand, due to the Pauli exclusion principle the occupation of the $p$-band is very convenient as long as the lowest $s$-band is fulfilled. In addition, the on-site attraction interaction can be enhanced by using atoms with large magnetic moments, such as $^{169}$Er with $m = 7\hbar_B$ on which laser cooling has been performed [27]. In contrast to [16,19], where a pair of extra lasers and a large magnetic field are needed to produce an effective SOC and split two SOC bands, respectively, our system is much simpler.

The organization of this paper is as follows. In the second section, we give the model and at the mean-field level investigate the ground state of the system by numerically minimizing the thermodynamic potential. In the third section by calculating the TKNN number $I_{TKNN}$ [28] of the occupied bands addressing the topological properties of the model, the topological phase diagram is obtained. In addition we also investigate the properties of edge states to prove our results. A brief conclusion is given in the fourth section.

Model and mean-field ground state. – The honeycomb optical lattice was realized experimentally by using three laser beams with co-planar propagating wave vectors quite some time ago [29]. It is well known that a honeycomb lattice is not a Bravais lattice and there are two inequivalent sites in a unit cell, denoted by A and B, respectively. Filling the lowest $s$-band and defining three unit vectors $\vec{e}_1 = \sqrt{\frac{3}{2}}\vec{e}_x + \frac{1}{\sqrt{2}}\vec{e}_y$, $\vec{e}_2 = -\sqrt{\frac{3}{2}}\vec{e}_x + \frac{1}{\sqrt{2}}\vec{e}_y$ and $\vec{e}_3 = \vec{e}_y$, the Hamiltonian of $p$-band honeycomb optical lattices with OSR is

$$H = t_{||} \sum_{\vec{r} \in A, i} \left[ \hat{p}_{\vec{r},\uparrow}^\dagger \hat{P}_{\vec{r} + \vec{e}_i, \downarrow} + H.c. \right] - \mu \sum_{\vec{r} \in A \oplus B} \hat{n}_{\vec{r}} - \Omega \sum_{\vec{r} \in A \oplus B} \hat{f}_{\vec{r}, z} - U \sum_{\vec{r} \in A \oplus B} \hat{p}_{\vec{r}, \downarrow}^\dagger \hat{p}_{\vec{r}, \downarrow} \hat{p}_{\vec{r}, \uparrow}^\dagger \hat{p}_{\vec{r}, \uparrow},$$

where $\hat{p}_{\vec{r}, \sigma} = (\hat{p}_{\vec{r}, \uparrow}^\dagger \hat{P}_{\vec{r}, \downarrow} + \hat{p}_{\vec{r}, \downarrow}^\dagger \hat{P}_{\vec{r}, \uparrow})$, $\hat{p}_{\vec{r}, x}$ and $\hat{p}_{\vec{r}, z}$ are the annihilation operator for the $p_x$ ($p_y$) band at the lattice site $\vec{r}$, $\hat{n}_{\vec{r}} = \hat{p}_{\vec{r}, \downarrow}^\dagger \hat{p}_{\vec{r}, \downarrow} + \hat{p}_{\vec{r}, \uparrow}^\dagger \hat{p}_{\vec{r}, \uparrow}$ and $\hat{f}_{\vec{r}, z} = -i(\hat{p}_{\vec{r}, \downarrow}^\dagger \hat{p}_{\vec{r}, \uparrow}^\dagger - \hat{p}_{\vec{r}, \uparrow}^\dagger \hat{p}_{\vec{r}, \downarrow}^\dagger)$ represent particle number and orbital-angular-momentum operators. $t_{||}$ is the nearest-neighbor hopping matrix element of atoms in $s$ bonds and positive due to the odd parity of the $p$-orbital.

When $U = 0$, by introducing the operator $\phi(k) = [p_{A\uparrow}(k), p_{A\downarrow}(k), p_{B\downarrow}(k), p_{B\uparrow}(k)]^T$ and making a unitary transformation $\phi_n(k) = U_{nm}(k)\Psi_m(k)$, the Hamiltonian can be diagonalized exactly. Meanwhile four energy bands can be obtained. We found that two of the four bands are always topological for any non-zero OSR and the others can be topological only if OSR is beyond a critical value [25]. On the basis of these findings, Wu proposed an orbital analogue of the quantum anomalous Hall effect, arising from orbital-angular-momentum polarization due to OSR. With $\Omega = 0$, Lee et al. discussed $f$-wave superfluidity and charge density wave (CDW) in this system at the mean-field level [24]. Their results show that away from the half-filling the system is $f$-wave superfluidity, while around the half-filling superfluidity and CDW coexist and the system is a supersolid. Although superfluidity exists all the time, it is not topological as stated below.

Following the same spirit in [24] we decouple the interaction term into CDW channel,

$$H_{int}^{CDW} = \sum_{\tau = x,y} \sum_{\vec{r} \in A} \left[ \frac{-n}{2} U + \frac{\Delta_{CDW}}{2} \right] \hat{p}_{\vec{r}, \tau}^\dagger \hat{p}_{\vec{r}, \tau} + \sum_{\vec{r} \in B} \left[ \frac{-n}{2} U + \frac{\Delta_{CDW}}{2} \right] \hat{p}_{\vec{r}, \tau}^\dagger \hat{p}_{\vec{r}, \tau}$$

and pairing channel

$$H_{int}^{p} = - \sum_k \left[ \Delta_{Ap} \hat{p}_{A\uparrow}(k) \hat{p}_{A\downarrow}^\dagger (-k) + \Delta_{Bp} \hat{p}_{B\uparrow}(k) \hat{p}_{B\downarrow}^\dagger (-k) + H.c. \right]$$

$$= - \sum_{k'} \left[ \Delta_{nm}(k) \Psi_n^\dagger (k') \Psi_m^\dagger (-k') + H.c. \right],$$

where $n = (\hat{n}_{\vec{r}, A} + \hat{n}_{\vec{r}, B})/2$ is the filling factor of every site, $\Delta_{CDW} = U(\hat{n}_{\vec{r}, A} - \hat{n}_{\vec{r}, B})/2$, $\Delta_{A} = U \sum_{k} \langle p_{A\downarrow}(k) p_{A\uparrow}(k) \rangle$, $\Delta_{B} = U \sum_{k} \langle p_{B\downarrow}(k) p_{B\uparrow}(k) \rangle$ are order parameters for CDW and superfluidity. In (3) we also express the pairing channel using the quasiparticle $\Psi(k)$. In this representation

$$\Delta_{nm}(k) = \Delta_{A} [U_{1n}^\dagger (k) U_{2n}^\dagger (-k) - U_{1n}^\dagger (k) U_{2n}^\dagger (-k)]$$

$$+ \Delta_{B} [U_{3n}^\dagger (k) U_{4n}^\dagger (-k) - U_{3n}^\dagger (k) U_{4n}^\dagger (-k)].$$

After the mean-field approximation, the Hamiltonian (1) becomes a BdG Hamiltonian $H = [\phi^\dagger (k), \phi (-k)] H_k [\phi (k), \phi^\dagger (-k)]^T$ and the properties of the
system are completely decided by the $8 \times 8$ matrix $H_k$. Diagonalizing $H_k$, we attain the spectra $\epsilon_i(k)$ and correspondingly eigenvectors $\varphi_i(k)$ ($i = 1, 2, \ldots, 8$). Due to particle-hole symmetry inherent in this BdG Hamiltonian, the spectra are symmetric about zero energy and we assume $\epsilon_1(k) = -\epsilon_8(k) > 0$, $\epsilon_2(k) = -\epsilon_7(k) > 0$, $\epsilon_3(k) = -\epsilon_6(k) > 0$, $\epsilon_4(k) = -\epsilon_5(k) > 0$. Then the thermodynamical potential at zero temperature is

$$F = \frac{1}{2} \sum_k [-4\mu - \epsilon_1(k) - \epsilon_2(k) - \epsilon_3(k) - \epsilon_4(k)]$$

$$+ \frac{N}{U} |\Delta_A|^2 + \frac{N}{U} |\Delta_B|^2 + \frac{N}{2U} \Delta_{CDW}^2,$$

where $N$ is the number of the unit cell. Below we numerically minimize the thermodynamic potential $F$ for $\Delta_A$, $\Delta_B$ and $\Delta_{CDW}$ for the fixed interaction strength $U$. Without loss of generality we choose $\Delta_A$ to be real, $\Delta_B = |\Delta_B| e^{i\theta}$ and $U/t_{||} = 3.0$.

Figure 1 shows the solutions of the Hamiltonian (1) at the mean-field level for changing chemical potential $\mu$ and OSR $\Omega$. Due to the particle-hole symmetry we only concentrate on negative chemical potential. Figure 1(a) describes the variation of $\Delta_{CDW}$. For $\Omega = 0$ CDW is robust, but when $\Omega$ is beyond a critical value $\Omega_c$, it suddenly vanishes. This is due to the fact that the appearance of OSR changes the band structures of single particle and breaks the nesting condition for CDW. Numerically we find $\Omega_c/t_{||} \approx 0.4$–0.6 and is monotonically increasing as the function of chemical potential. Figure 1(b) shows the effect of OSR on particle density and further exemplifies that the variations of band structures driven by OSR cause non-monotonic behavior of particle density. In contrast, superfluid order parameters $\Delta_A$, $\Delta_B$ are more interesting and shown in panels (c) and (d). On the one hand, for $\Omega > \Omega_c$, $\Delta_A = |\Delta_B|$ and with the increase of OSR, superfluid order smoothly decreases until disappearance. This suppression mechanism of superfluidity consists in time-reversal symmetry breaking caused by OSR. While, on the other hand, for $\Omega < \Omega_c$, $\Delta_A$ is still decreasing but $\Delta_B$ is increasing with $\Omega$. In fact the increase of $\Delta_B$ originates from the redistribution of particle density between sites A and B, in other words the decrease of $\Delta_{CDW}$ as seen in panel (a). Thus, at the mean-field level our calculation suggests that 1) OSR weakens the stabilities of CDW and superfluidity and 2) for $\Omega < \Omega_c$, superfluidity and CDW coexist and the system is a supersolid.

The optimization of $\theta$ leads to $\theta = \pi$ for all parameters we choose. Below we discuss the effects of OSR on pairing symmetry for $\Omega > \Omega_c$. From [24] without OSR and away from the half-filling the intraband pairings in (4) have $f$-wave symmetry with three nodal lines of $k_x = 0$, $k_y = \pm k_x \sqrt{3}$ and $\pi/3$ rotation symmetry (fig. 2(d)). When $\Omega > \Omega_c$, (4) can be written into $\Delta_{nm}(k) = \Delta_A f_{nm}(k)$ due to $\Delta_A = -\Delta_B$. In terms of the pairing magnitude, nodal lines degenerate into some disconnected regions where the

Fig. 1: (Color online) The mean-field solution of the Hamiltonian (1). Parameter $U/t_{||} = 3.0$. 

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Fig. 2: (Color online) The symmetry of intraband pairing $f_{11}$. In (a) the magnitude, (b) real part and (c) imaginary part of $\Delta_{11}$ for $\Omega/t_\| = 1.0$ are shown. For comparison panel (d) plots $f_{11}$ for $\Omega/t_\| = 0$.

Fig. 3: (Color online) Topological phase diagram of the Hamiltonian (1) at the mean-field level. The light grey, dark grey, black and blue colors correspond to $I_{TKNN} = 1, 0, -1, 2$, respectively. Parameter $U/t_\|=3.0$.

intraband gap disappears, and $\pi/3$ rotation symmetry remains (fig. 2(a)), while the real and imaginary parts of pairing break $\pi/3$ into $\pi$ rotation symmetry (fig. 2(b) and (c)). Although intraband gaps disappear in certain regions of the Brillouin zone, due to the multiband structure, the superfluid state remains fully gapped.

Topological phase diagram and Majorana fermion modes. – In this section we discuss the topological properties of the Hamiltonian (1). In terms of our system, it explicitly breaks the time-reversal symmetry due to OSR. Thus, the TKNN number $I_{TKNN}$ plays a central role in deciding the topological nature of the system [28]. The TKNN number is defined by eigenvectors $\varphi_i(k)$ ($i = 5, 6, 7, 8$) corresponding to the negative energy spectrum of the matrix $H_k$, into $I_{TKNN} = \frac{1}{2\pi} \int d^2k Tr A$, where $A$ is a matrix one-form $A_{ij} = A_{ij}^\nu dk_\nu$ with $A^\nu_{ij}(k) = \varphi_i^\nu(k)\nabla_k^{\nu} \varphi_j(k)$. By numerically calculating the TKNN number [30], we show the topological phase diagram of the system in fig. 3. For the parameter region we choose, there are four different subregions labeled by $I_{TKNN} = 1, 0, -1, 2$, respectively. Moreover by comparison with fig. 1(a) it is easily found that the boundary between $I_{TKNN} = 0$ and other TKNN numbers in the direction of $\Omega$ coincides with that of the CDW disappearance. This finding is very important and ensures that the topological order of our system is not topological CDW [31]. According to the criteria for TS [31] $I_{TKNN} = 2$ corresponds to Abelian TS, while $I_{TKNN} = 1, -1$ are non-Abelian TSs. Thus, fig. 3 tells us that OSR drives topological phase transition not only from NS to TS, but also between different TSs. Here we mention the fact that the energy gap of the bulk spectrum closes when topological phase transitions between topologically distinct phases occur.

From the bulk-edge correspondence, a non-trivial bulk topological number implies the existence of gapless edge states localized on open edges of the system. Cold Fermi
gases with sharp edges may be realized along the lines proposed in [32]. In order to understand the relation between $I_{TKNN}$ and the number of edge states, we study the Hamiltonian (1) with the open boundary condition along the zigzag edge of the honeycomb lattice. The resulting excitation spectrum are depicted in fig. 4 for representative parameter choices. Very explicitly the number of gapless states for every edge has one-to-one correspondence with the TKNN number. For $I_{TKNN} = \pm 1$ ($I_{TKNN} = 2$) there are one (two) pair(s) of gapless states, while for $I_{TKNN} = 0$, the gapless state does not exist. Due to particle-hole symmetry, in terms of gapless states, they are Majorana fermion modes. It should also be remembered that the core of a vortex is topologically equivalent to an edge which has been closed on itself. The edge modes we describe are therefore equivalent to the Majorana fermions known to exist in the core of vortices of $p$-wave superfluids [33].

**Conclusions.** – In conclusion, at the mean-field level we have investigated the effects of OSR on CDW and superfluidity for $p$-band spinless Fermi gases in honeycomb optical lattices. We found that OSR weakens the stabilities of CDW and superfluidity simultaneously, although superfluidity can survive a larger OSR. This conclusion leads to another important result, i.e., that once CDW drops out, the system enters into topological superfluidity. By numerically calculating the TKNN number we obtained the topological phase diagram of the system. In addition edge states, i.e., bulk-boundary correspondence, are also investigated.

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Fig. 4: (Color online) The gapless edge states with the open boundary condition along the zigzag edge of the honeycomb lattice. (a) $I_{TKNN} = 0$, $\mu/t_1 = -0.75$, $\Omega/t_1 = 0.3$, $\Delta_A/t_1 = 0.969$, $\Delta_B/t_1 = 0.063$, $\Delta_{CDW}/t_1 = 1.462$; (b) $I_{TKNN} = 2$, $\mu/t_1 = -0.5$, $\Omega/t_1 = 0.8$, $\Delta_A/t_1 = \Delta_B/t_1 = 0.288$, $\Delta_{CDW}/t_1 = 0$; (c) $I_{TKNN} = -1$, $\mu/t_1 = -0.85$, $\Omega/t_1 = 0.8$, $\Delta_A/t_1 = \Delta_B/t_1 = 0.523$, $\Delta_{CDW}/t_1 = 0$; (d) $I_{TKNN} = 1$, $\mu/t_1 = -0.65$, $\Omega/t_1 = 1.1$, $\Delta_A/t_1 = \Delta_B/t_1 = 0.307$, $\Delta_{CDW}/t_1 = 0$. 

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