The competition between the intrinsic and Rashba spin–orbit coupling and effects of correlations on Rashba SOC-driven transitions in the Kane–Mele model

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Abstract

We investigate, firstly, the competition between the Rashba spin–orbit coupling (SOC) and the intrinsic SOC in Kane–Mele model. For the small intrinsic SOC, we investigate the effects of the Rashba SOC on the touching point of the valence and conduction bands when the ratio of the Rashba SOC to the intrinsic SOC is greater than classical value $2\sqrt{3}$. For the large intrinsic SOC, we find that the critical ratio of the two SOCs at which the band touching occurs decreases with the increasing intrinsic SOC and the locations of these touching points deviate from points $K$ and $K'$ of the Brillouin zone. Furthermore, effects of the Rashba SOC on these touching points are discussed in detail when the ratio is greater than the critical value. The Rashba SOC-driven topologically trivial and non-trivial transitions are also obtained in the first part of the work. Secondly, using the slave-rotor mean field method we investigate the influences of the correlation on the Rashba SOC-driven topologically trivial and non-trivial transitions in both the charge condensate and Mott regions. The topological Mott insulator with gapped or gapless spin excitations which arises from the interplay of the Rashba SOC and correlations is obtained in the work.

Keywords: Kane–Mele model, Rashba SOC-driven transition, strong correlations, slave-rotor mean field method

(Some figures may appear in colour only in the online journal)

1. Introduction

Over the past few decades, topological insulators have attracted a lot of attentions from the condensed matter community, owing to its topologically non-trivial insulating band [1, 2]. From a mathematical perspective, the novel structure of bands stems from the non-zero (actually an integer) consequence of the integral of the Berry curvature over one half of the Brillouin zone (BZ) or the integral winding number of the mapping from the Brillouin torus onto the space of the Bloch Hamiltonian (a two-sphere) [3–6]. The non-trivial consequence of the insulating band implies that systems with changing model parameters belong to the same topological class in which these systems are adiabatically interconnected as long as the band gap stays open. In other words, a topological insulating class possessed by the system can turn into the another one and the topological transition occurs when the direct energy gap of a system closes. A significant toy model of topological insulators is the famous Kane–Mele (KM) model on the honeycomb lattice proposed by Kane and Mele in 2005 [7], and soon after its non-trivial band structure was characterized by the $Z_2$ topological invariant [8]. The non-trivial band structure of the model arises from the intrinsic spin–orbit coupling (SOC) of next-nearest neighbor
(NNN) electrons. Although the time-reversal symmetry of the model is guaranteed by the intrinsic SOC, the symmetry is actually broken for each spin. Then, the KM model can be thought of as two copies of the Haldane model [9] with opposite Chern numbers. It is the breaking of time-reversal symmetry of each spin sector that leads to the non-trivial consequence of the integral of the Berry curvature over the BZ in the KM model. Although the experimental observation of the topologically non-trivial insulating band possessed by the KM model has not been achieved due to the tiny magnitude of the intrinsic spin–orbit gap of graphene [10], the one possessed by the Bernevig–Hughes–Zhang model has been experimentally realized in the CdTe/HgTe/CdTe quantum well [11, 12].

Besides the intrinsic SOC, there is a so-called extrinsic SOC in 2D mesoscopic systems, i.e. the Rashba SOC [13, 14]. It can arise due to the presence of external electric fields [14], a substrate [15] or neutral impurities [16, 17]. The effects of the Rashba SOC on the band of electrons in the graphene sheet have been investigated in detail [18, 19]. The extrinsic SOC cannot open a gap in the energy band and maintains Dirac nodes of the original tight-binding model of electrons in the graphene sheet. However, the spin degeneracy of each band is lifted due to the breaking of mirror symmetry, and then the Rashba SOC can force the electron in the graphene sheet to possess two zero-gap bands and two gapped bands. Furthermore, it is clear that the electron spin polarizations of all bands are in the $(k_x, k_y)$-plane of momentum and they are perpendicular to momentum $k$ if the Rashba SOC is isotropic. Thus, it is interesting to observe what happens when the Rashba SOC is introduced into the KM model—the electron model in the graphene sheet with the intrinsic SOC which always possesses gapped spin-degenerate bands. Besides the splitting of bands, the Rashba SOC can remove the direct band gap caused by the intrinsic SOC if its strength is large enough [20]. This remarkable consequence of the competition between the intrinsic SOC and the Rashba SOC is the destruction of the topologically non-trivial insulating band [8, 21, 22], i.e. the Rashba SOC can drive the KM model into a topologically trivial state from the $Z_2$ topological insulator. However, we suppose that the competition between the two SOCs in the KM model has not been explored fully. For example, the deformation of the band caused by the Rashba SOC can lead to the shift of the touching point of the valence band and conduction band where the direct band gap closes and then the topological non-trivial transition occurs. Furthermore, the splitting of this touching point due to the crossing of the valence band and the conduction band have not been investigated yet. In the first part of our study, the effects of Rashba SOC on the band structure of KM model which have not been exposed entirely will be discussed in detail and the Rashba SOC-driven topologically trivial or non-trivial phase transition derived here will be applied in the second part of our study.

For the topologically non-trivial insulating band, a natural and important question arises. To what extent is its structure stable against electron correlations and then what kinds of novel states can arise from the interplay between topology and electron correlations? Effects of electron correlations on topologically non-trivial insulating bands had already been investigated by several authors in the early years of topological insulators [7, 23, 24]. The conclusion is that the topologically non-trivial insulating band is stable against the weaker electron correlation or disorder as long as they leave the gap open. The two earlier investigations of effects of the stronger electron correlation on topologically non-trivial insulating bands were, in our opinion, given by Young et al [25] using the slave-rotor mean field theory and Cai et al [26] using the Hartree–Fock mean field method. Since then, there have been a large number of discussions on the effects of strong correlations on topological bands [27–29]. Let us focus on effects of strong correlations on the KM model on the honeycomb lattice. It has been investigated by various analytical or numerical methods, e.g. slave-particle/spin mean field theories [25, 30, 31], Schwinger boson/fermion approaches [32], the cellular dynamical mean field theory [33], the variational cluster approach (VCA) [34] and the quantum Monte Carlo (QMC) simulation [35–37]. In general, the topologically non-trivial insulating band of the KM model is stable against the weaker correlations and the magnetic insulating phase which may destroy the topological structure of bands can emerge when the correlations become sufficiently strong. In the case of intermediate correlations, the topologically non-trivial structure of bands is maintained and various exotic states which stem from the interplay of topology and correlations, e.g. the topological Mott insulator (TMI), the quantum spin liquid (QSL), and the quantum spin Hall (QSH) state coupled to a dynamical $Z_2$ gauge field (QSH$^*$), can emerge. Some of phase transitions in the correlated KM model have been investigated by Hohenadler et al [37] using the QMC simulation and Griset and Xu [38] from the viewpoint of field theory. Furthermore, Bercx et al [39] have investigated effects of strong correlations on the KM model on the honeycomb lattice with a magnetic flux of $\pm \pi$ through each hexagon. They found that the antiferromagnetic order develops above a critical value of the correlation, which is similar to the case of the ordinary correlated KM model, and there is a correlation-induced gap in the edge states as a result of umklapp scattering at half-filling.

Let’s return to effects of the Rashba SOC in the case of electron correlations. At present, the investigations focus mainly on effects of the Rashba SOC on the edge states of topological insulators with correlation, e.g. effects on the electron backscattering [40–42] and spin correlations and spectral gap [43] of correlated helical edge states. For the bulk of topological insulators, Laubach et al [44] reported, applying the VCA, a new topological–semiconductor phase which stems from the Rashba SOC in the Kane–Mele–Hubbard (KMH) model, and Mishra and Lee [45] sketched out the effects of the Rashba SOC on the phase diagram of interacting KM model at quarter filling. In the first part of our study, the competition between the intrinsic SOC and the Rashba SOC has been investigated. We want to know more effects of electron correlations on the bulk of topological insulators with the Rashba SOC, especially
on the Rashba SOC-driven topologically trivial or non-trivial phase transition. It is well known that the strong correlation can lead to a spin-charge separation where the charge degree of freedom is uncondensed and the spin degree of freedom may form a spin liquid state. In this work, focusing on the correlated KM model with the Rashba SOC, we will consider both of the spin-charge separation caused by the strong correlation and the topologically trivial or non-trivial phase transition driven by the Rashba SOC, and then investigate the influences of electron correlations on the Rashba SOC-driven phase transition in the condensate and Mott region of charge degree of freedom respectively.

Our paper is organized as follows. In section 2, we revisit the KM model with the Rashba SOC. The competition between the two SOCs is investigated in detail and the Rashba SOC–Hubbard interaction is introduced into the model and the honeycomb lattice is

2. The KM model with the Rashba SOC

2.1. The model

The KM model with the Rashba SOC (R–KM model) on the honeycomb lattice is

\[
H_0 = -t \sum_{\langle ij \rangle} \sum_\sigma \hat{c}^\dagger_i \sigma \mathbf{\hat{a}}_{ij} \sigma \hat{c}_j + i \lambda \sum_{\langle ij \rangle} \sum_{\sigma \sigma'} \nu_{ij} \hat{c}^\dagger_i \sigma \sigma' \mathbf{\hat{a}}_{ij} \sigma' \hat{c}_{j \sigma'} + i \alpha \sum_{\langle ij \rangle} \sum_{\sigma \sigma'} \hat{c}^\dagger_i (\sigma \sigma' \times \mathbf{d}_{ij}) \hat{c}_{j \sigma'}. \tag{1}
\]

Here the first term is the nearest neighbor (NN) electrons hopping term with the hopping strength \( t \). The second term represents the intrinsic SOC between NN electrons with the coupling strength \( \lambda \). \( \sigma \sigma' \) is the \( z \) component of Pauli matrices and the parameter \( \nu_{ij} = -1 \) if the orientation of the NN sites \( i, j \) is right turn while \( \nu_{ij} = +1 \) if left turn. The third term is the Rashba SOC term of NN electrons with coupling strength \( \alpha \) and \( \mathbf{d}_{ij} \) is the connected vector from site \( i \) to site \( j \). Lattice vectors of the honeycomb lattice are \( \mathbf{a}_1 = (3a/2, \sqrt{3}a/2) \) and \( \mathbf{a}_2 = (3a/2, -\sqrt{3}a/2) \), as shown in figure 1. In the concrete calculation, we set the lattice constant \( a = 1 \) and the strength of NN hopping \( t = 1 \).

In momentum space, the Hamiltonian of R–KM model can be obtained as

\[
H_0 = \sum_k \Psi_k^\dagger H_0 \Psi_k. \tag{2}
\]

Here \( \Psi_k = (\hat{c}_k^A, \hat{c}_k^B, \hat{c}_k^A, \hat{c}_k^B)^T \) is the matrix of electron operators in the momentum–spin space and the Bloch Hamiltonian

\[
H_{0k} = \begin{pmatrix}
\lambda \gamma & -tg & 0 & \alpha(w_j - iw_j) \\
-tg & -\lambda \gamma & \alpha(w_i - iw_i) & 0 \\
0 & \alpha(w_i + iw_i) & -\lambda \gamma & -tg \\
\alpha(w_i^* + iw_i^*) & 0 & -tg^* & \lambda \gamma
\end{pmatrix}, \tag{3}
\]

where \( A, B \) represent the sublattice of the honeycomb lattice as shown in figure 1, \( g = \sum_i e^{i \mathbf{k} \mathbf{d}_i}, \mathbf{w}_x = \text{sgn}(\sqrt{3}ak_x) + 2 \cos(3ak_x/2) \sin(\sqrt{3}ak_x/2) \) and \( \gamma = 2[\text{sgn}(\sqrt{3}ak_x) + 2 \cos(3ak_x/2) \sin(\sqrt{3}ak_x/2)]. \)

2.2. The competition between the intrinsic and Rashba SOC and Rashba SOC-driven transitions

It is the non-zero elements at counter-diagonal of Hamiltonian matrix \( H_{0k} \) that mix the up-spin and down-spin and violate mirror symmetry, and then lift the spin degeneracy of bands and break the particle–hole symmetry of bands. Although these terms prevent us from diagonalizing the Hamiltonian by hand easily, the band energy and eigenstates of bands can be obtained numerically or analytically by computer.

For \( \lambda = 0 \) and \( \alpha = 0 \), the energy band is just the one of electrons with the spin in the graphene sheet, which is gapless and has Dirac nodes at \( K(2\pi/3, 2\pi/3\sqrt{3}a) \) and \( K'(0, 4\pi/3\sqrt{3}a) \) in the BZ. For \( \lambda = 0 \) and \( \alpha \neq 0 \), the Rashba SOC lifts the spin degeneracy of bands and keeps the energy spectrum gapless. For \( \lambda \neq 0 \) and \( \alpha = 0 \), bands of the KM model have the spin degeneracy and the intrinsic SOC always opens energy gaps at \( K \) and \( K' \). The previous results are well known in the graphene research community. The case of \( \lambda \neq 0 \) and \( \alpha \neq 0 \) where the Rashba SOC competes with the intrinsic SOC will be investigated as follows. In our discussions, a ratio \( \chi = \frac{\alpha}{\lambda} \).

Firstly, let us focus on the case of the small intrinsic SOC. There are two well-known facts. One is that when the Rashba SOC increases gradually, besides the lifting of the spin degeneracy of bands, the band gap decreases and the touching of the valence band and the conduction band occurs eventually. It is clear that the touching points are located at \( K \) and \( K' \) in the BZ. The famous result [8] of the critical value of Rashba SOC at which the band touching or the topologically non-trivial transi-
a Rashba SOC-driven topologically trivial transition from the rect gap of the valence band and conduction band closes and touching points for all of the three red points represent the locations of touching points when $\alpha = \chi_{\text{topo}} \cdot \lambda$, where $\chi_{\text{topo}} = \chi_0 = 2\sqrt{3}$. Beyond the transition, the system stays in a topologically trivial metal phase because of the band touching and has more band touching points which are split from the ones at $K$ and $K'$ due to the dominance of the Rashba SOC.

However, this is not the full story. The missing piece can be retrieved from the investigation of the band touching of the valence and conduction bands at large intrinsic SOCs. It is also a fact that the band touching at $K$ and $K'$ always occurs when the Rashba SOC $\alpha = \chi_0 \lambda$ ($\chi_0 = 2\sqrt{3}$). Therefore, the larger the intrinsic SOC is, the larger Rashba SOC is needed to develop this type of band touching. On the other hand, the large Rashba SOC can greatly ‘enhance’ the crossing of bands which causes the additional band touching. Thus it is possible that the additional band touching which differs from the one at $K$ or $K'$ can occur before the Rashba SOC reaches the critical value of $\chi_0\lambda$. The process in the case of $\lambda = 0.4$ is shown in the figure 3. At the critical Rashba SOC $\alpha = \chi_{\text{topo}} \cdot \lambda$ ($\chi_{\text{topo}} \approx 2.903 < \chi_0$), the band touching occurs at some points who differ from the $K$ and $K'$. These locations of band touching points in BZ also possess the 2$\pi$/3 rotational symmetry as shown in figure 3(a). Here we write the critical $\chi$ as $\chi_{\text{topo}}$, because the band touching implies a topologically non-trivial transition due to the closing of the direct band gap. Beyond this critical Rashba SOC, the model stays in the topologically trivial metal state and the effect of the Rashba SOC is just to split and shift the touching points (see below). When the Rashba SOC increases further ($\chi > \chi_{\text{topo}}$), touching points are split because of the band crossing as shown in figure 3(b). The inside points move toward the $K$ or $K'$ with the increasing Rashba SOC. Eventually, a touching point forms at $K$ or $K'$ when $\chi = \chi_0$ and there are three satellite touching points around the single point, which is similar to the case of small intrinsic SOCs, e.g. $\lambda = 0.1$. The case of $\chi = \chi_0$ is shown in figure 3(c). The further increasing Rashba SOC enforces satellite touching points to move away from points $K$ or $K'$ and maintains the single touching point at the $K$ or $K'$ as shown in figure 3(d).

For the small Rashba SOC ($\chi < \chi_{\text{topo}}$), the intrinsic SOC dominates and the model possesses topologically non-trivial states. There is also a Rashba SOC-driven topologically trivial transition from the $Z_2$ topological insulator to the TSM occurs. The topologically non-trivial phase keeps until the band touching occurs at points $K$ and $K'$. The Rashba SOC-driven topologically non-trivial transition (or band touching) occurs when the Rashba SOC reaches the second critical value $\alpha = \chi_{\text{topo}} \cdot \lambda$, where $\chi_{\text{topo}} = \chi_0 = 2\sqrt{3}$. Beyond the transition, the system stays in a topologically trivial metal phase because of the band touching and has more band touching points which are split from the ones at $K$ and $K'$ due to the dominance of the Rashba SOC.
Figure 3. Locations of touching points of the valence band and the conduction band in BZ at \( \lambda = 0.4 \) in the case of \( \chi \geq \chi_{\text{topo}} \approx 2.903 \). (a) \( \chi = \chi_{\text{topo}} \), (b) \( \chi_{\text{topo}} < \chi < \chi_0 \), (c) \( \chi = \chi_0 \) and (d) \( \chi > \chi_0 \). The blue dotted triangles are used to mark out the locations of touching points around the \( K \) and \( K' \).

Figure 4. Critical value of ratio \( \chi = \alpha / \lambda \) at which the topologically trivial or non-trivial transition occurs. For small enough intrinsic SOC, the \( \chi_{\text{topo}} = 2\sqrt{3} \) as the classical result.

Figure 5. The phase diagram of the R–KM model. Z, Z\(_2\) TI: \( Z_2 \) topological insulator, TSM: topological semi-metal and M: metal. The critical value \( \chi_{\text{topo}} = \chi_0 = 2\sqrt{3} \) for the smaller intrinsic SOC and \( \chi_{\text{topo}} < \chi_0 \) for the larger one. The variation of \( \chi_{\text{topo}} \) or \( \chi_{\text{ntopo}} \) with the increasing intrinsic SOC was shown in figure 4.

3. The R–KM model with strong correlations

In the section, the strong correlation represented by the on-site Hubbard interaction is introduced into the R–KM model (called R–KMH model). Strongly correlated systems can display the spin-charge separation. It postulates that the electron in these systems can be viewed as a composite of the chargon and the spinon. The slave-rotor representation of the physical electron operators can treat economically the spin-charge separation and describe appropriately the Mott transition of the charge degree of freedom in the region of intermediate correlations [47–49]. It is well known that the correlation can renormalize model parameters of a system and then change the physical quantities of the system. In the slave-rotor mean field method the benefit is that the spin degree of freedom (i.e. the spinon) inherits the Hamiltonian of physical electrons, but with the renormalized model parameters, e.g. the renormalized intrinsic or Rashba SOC in our studied model here. In the preceding section we obtained the Rashba SOC-driven topologically trivial and non-trivial transition. Therefore, it is interesting to observe what happens to the Rashba SOC-driven transition when the R–KM model is renormalized by the correlation. Here we capture the Mott transition of the charge degree of freedom at the intermediate Hubbard interaction using the slave-rotor mean field method. The boundary of the Mott transition is obtained numerically from the mean field self-consistency equations in this section. Furthermore, the slave-rotor mean field method will be applied to obtain Rashba SOC-driven topologically trivial and non-trivial transitions in both cases of condensed and uncondensed charges. We will compare these results with the ones in the case of non-interacting limit. The influences of correlations on the Rashba SOC-driven topologically trivial and non-trivial transitions in regions of condensed charge (i.e. physical electron) and uncondensed charge (i.e. spinon) are discussed in detail here.

3.1. The slave-rotor mean field method for correlated R–KM model

3.1.1. Slave-rotor representation for the correlated model. When the on-site Hubbard term is introduced, the Hamiltonian of the R–KMH model reads

\[
H = H_0 + \frac{U}{2} \sum_i \left( \sum_{\sigma} n_{i\sigma} - 1 \right)^2 .
\]  

(4)

Here \( H_0 \) is given by equation (1) and \( n_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \) is the number operator of electrons with spin-\( \sigma \).

The slave-rotor representation [47–49] decomposes the annihilation operator of the physical electron as

\[
\hat{c}_{i\sigma} = e^{\psi_\sigma} \hat{f}_{i\sigma}.
\]  

(5)

Here \( e^{\psi_\sigma} \) is the \( U(1) \) rotor operator that describes the charge degree of freedom and \( \hat{f}_{i\sigma} \) is the spinon operator that describes the spin degree of freedom of the electron. There is a constraint that recovers the Hilbert space of the electron...
\[
\sum_{\sigma} \tilde{f}_{\sigma}^\dagger \tilde{\hat{f}}_{\sigma} + \hat{L}_i = 1.
\]

(6)

where the canonical angular momentum \( \hat{L}_i = i \partial \theta_i \) associated with the angular \( \theta_i \) is introduced.

The model Hamiltonian can be written in the rotor and spinon operators as

\[
\begin{align*}
H &= -\sum_{\langle ij \rangle, \sigma} e^{-i \theta_{ij}} \tilde{f}_{\sigma}^\dagger \tilde{\hat{f}}_{\sigma'}^\dagger \hat{f}_{\sigma'} \hat{f}_{\sigma'}^\dagger \hat{f}_{\sigma}^\dagger f_{\sigma}^\dagger f_{\sigma} + i \lambda \sum_{\langle ij \rangle, \sigma} \nu_{ij} e^{-i \theta_{ij}} \tilde{f}_{\sigma}^\dagger \hat{f}_{\sigma'}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma'}^\dagger \hat{f}_{\sigma}^\dagger f_{\sigma}^\dagger f_{\sigma}^\dagger f_{\sigma} + U \sum_{i} \hat{L}_i^2 - \mu \sum_i \tilde{f}_{\sigma}^\dagger \tilde{\hat{f}}_{\sigma}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma}.
\end{align*}
\]

(7)

Here, \( \theta_{ij} = \theta_i - \theta_j \), and \( \mu \) is the chemical potential. The partition function of the system is written as a path integral of \( e^{-\beta E} \) over fields \( f, \tilde{f} \) and \( \theta \), where

\[
S_E = \int_0^\beta d\theta \left[ \sum_i -i \eta \partial_i \theta_i + \sum_{\langle ij \rangle, \sigma} f_{\sigma}^\dagger \partial_i f_{\sigma} + \sum_{\langle ij \rangle, \sigma} \nu_{ij} \tilde{f}_{\sigma}^\dagger \sigma_{\sigma'} \times d_{ij} \tilde{\hat{f}}_{\sigma}^\dagger \hat{f}_{\sigma'}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma} + \frac{\lambda}{2} \sum_{\langle ij \rangle, \sigma} \nu_{ij} \tilde{f}_{\sigma}^\dagger \sigma_{\sigma'} \hat{f}_{\sigma'}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma} + \frac{1}{2U} \sum_i \left( \partial_i \theta_i + i \eta \right)^2 - \sum_i \tilde{f}_{\sigma}^\dagger \tilde{\hat{f}}_{\sigma}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma} + \frac{\lambda}{2} \sum_{\langle ij \rangle, \sigma} \nu_{ij} \tilde{f}_{\sigma}^\dagger \sigma_{\sigma'} \times d_{ij} \tilde{\hat{f}}_{\sigma}^\dagger \hat{f}_{\sigma'}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma}^\dagger f_{\sigma}^\dagger f_{\sigma} + \frac{1}{2U} \sum_i \left( \partial_i \theta_i + i \eta \right)^2 \right]
\]

(8)

Here, the symbol ‘\( \cdots \)’ denotes constant terms of mean field decomposition and we have set \( \hbar_i \equiv h = -\mu = 0 \) for half-filling at the mean field level. \( \rho_i \) is the Lagrange multiplier for constraint \( \sum_{\langle ij \rangle} f_{\sigma}^\dagger f_{\sigma} = 1 \) and \( \rho_i \equiv \rho \) in the mean field treatment. In the above expression,

\[
H^X = -tQ_X \sum_{\langle ij \rangle} X_i^* X_j + \lambda Q^X \sum_{\langle ij \rangle} X_i X_j
\]

\[
\left( \langle \partial_i \theta_i + i \eta \rangle - i \sum_{\langle ij \rangle, \sigma} \nu_{ij} \tilde{f}_{\sigma}^\dagger \sigma_{\sigma'} \times d_{ij} \tilde{\hat{f}}_{\sigma'}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma} + \frac{1}{2U} \sum_i \left( \partial_i \theta_i + i \eta \right)^2 \right)
\]

(9)

It is more convenient to introduce a new field \( X_i = e^{i \theta_i} \) to represent the charge degree of freedom. The new field satisfies the constraint \( |X_i|^2 = 1 \) due to its complex exponential form. Furthermore, to express the action in quadratic form of \( X \)-field and \( f \)-field five mean field parameters should be introduced:

\[
Q_X = \left( \sum_{\langle ij \rangle} f_{\sigma}^\dagger f_{\sigma} \right),
\]

(10)

The action can be obtained as

\[
S_E = \int_0^\beta d\tau \left[ \sum_i -i \partial_i \theta_i + \sum_{\langle ij \rangle, \sigma} f_{\sigma}^\dagger \partial_i f_{\sigma} + \sum_{\langle ij \rangle, \sigma} \nu_{ij} \tilde{f}_{\sigma}^\dagger \sigma_{\sigma'} \times d_{ij} \tilde{\hat{f}}_{\sigma'}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma} + \frac{1}{2U} \sum_i \left( \partial_i \theta_i + i \eta \right)^2 \right]
\]

(11)

Here, \( \beta \) is the symbol ‘\( \cdots \)’ denotes constant terms of mean field decomposition and we have set \( \hbar_i \equiv h = -\mu = 0 \) for half-filling at the mean field level. \( \rho_i \) is the Lagrange multiplier for constraint \( \sum_{\langle ij \rangle} f_{\sigma}^\dagger f_{\sigma} = 1 \) and \( \rho_i \equiv \rho \) in the mean field treatment. In the above expression,

\[
H^X = -tQ_X \sum_{\langle ij \rangle} X_i^* X_j + \lambda Q^X \sum_{\langle ij \rangle} X_i X_j
\]

(12)

\[
Q^X = \left( \sum_{\langle ij \rangle} \nu_{ij} \tilde{f}_{\sigma}^\dagger \sigma_{\sigma'} \times d_{ij} \tilde{\hat{f}}_{\sigma'}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma} + \frac{1}{2U} \sum_i \left( \partial_i \theta_i + i \eta \right)^2 \right)
\]

(13)

\[
Q^X = \left( \sum_{\langle ij \rangle} \nu_{ij} \tilde{f}_{\sigma}^\dagger \sigma_{\sigma'} \times d_{ij} \tilde{\hat{f}}_{\sigma'}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma} + \frac{1}{2U} \sum_i \left( \partial_i \theta_i + i \eta \right)^2 \right)
\]

(14)

\[
Q^X = \left( \sum_{\langle ij \rangle} f_{\sigma}^\dagger (\sigma_{\sigma'} \times d_{ij} \tilde{f}_{\sigma'}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma}) \right)
\]

(15)

Here, the symbol ‘\( \cdots \)’ denotes constant terms of mean field decomposition and we have set \( \hbar_i \equiv h = -\mu = 0 \) for half-filling at the mean field level. \( \rho_i \) is the Lagrange multiplier for constraint \( \sum_{\langle ij \rangle} f_{\sigma}^\dagger f_{\sigma} = 1 \) and \( \rho_i \equiv \rho \) in the mean field treatment. In the above expression,

\[
H^X = -tQ_X \sum_{\langle ij \rangle} X_i^* X_j + \lambda Q^X \sum_{\langle ij \rangle} X_i X_j
\]

(16)

\[
Q^X = \left( \sum_{\langle ij \rangle} \nu_{ij} \tilde{f}_{\sigma}^\dagger \sigma_{\sigma'} \times d_{ij} \tilde{\hat{f}}_{\sigma'}^\dagger \hat{f}_{\sigma} \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma} + \frac{1}{2U} \sum_i \left( \partial_i \theta_i + i \eta \right)^2 \right)
\]

(17)

The action of equation (15) can be transformed into frequency–momentum space via Fourier transforms

\[
X_\omega(\tau) = \frac{1}{\sqrt{\beta N_A}} \sum_{k,n} e^{ik\cdot R - in\tau} X_k(\nu_n) + \sqrt{\nu_0},
\]

(18)

\[
f_{\sigma}(\omega) = \frac{1}{\sqrt{\beta N_A}} \sum_{k,n} e^{ik\cdot R - in\tau} f_{k\sigma}(\nu_n)\omega_k.
\]

(19)

Here \( N_A \) denotes the number of unit cells and \( \nu_0 \) is the condensate density of charges. \( \nu_n = 2n\pi / \beta \) are the Matsubara frequencies for bosons and \( \omega_n = (2n + 1)\pi / \beta \) for fermions and the summation excludes the point \( (\nu_n, k^\dagger) \) at which the condensate of charges occurs. Finally, we can write the action in matrix form as

\[
S_E = \sum_{k,n} \Psi^{X \dagger}_{\eta} \left( \frac{\nu_n^2}{2U} + \rho \right) \delta_{\eta k} + H^X \Psi^X \Psi^X_k + \sum_{k,n} \Psi_{\eta}^{f \dagger} \left( -i\omega_\eta \right) \delta_{\eta k} + H^{f \dagger} \Psi_{\eta}^f + \cdots
\]

(20)
3.1.2. Green’s functions and self-consistency equations of two degrees of freedom.

The Green’s function of the charge degree of freedom in the lower band (i.e., valence band) can be obtained from the action of equation (20) using the standard formulae [50]. We get

\[ G^1_X = \frac{1}{\nu_n U + \rho + E^1_X} \hspace{1cm} (23) \]

Here \( E^1_X = -| - iQ_X + \alpha Q'_X|g + \lambda Q'_X \gamma X \) is the lower eigenenergy of the Hamiltonian matrix \( H^X \) of the X-field. Similarly, the Green’s functions of the spinon in the two lower bands can be obtained as

\[ G^{(2)}_f = \frac{1}{\nu_n - E^{(2)}_f} \hspace{1cm} (24) \]

Here \( E^{(1)}_f \) and \( E^{(2)}_f \) are the two lower eigenenergies of the Hamiltonian matrix \( H^f \). Although it is actually not so easy to diagonalize the matrix \( H^f \) by hand, the eigenenergy \( E_f \) and eigenvectors required for the mean field equations (see below) can be obtained more easily by computer both analytically and numerically. The pole of the Green’s function in the imaginary frequency domain gives the energy spectra of bands. Therefore, energy spectra of the charge and spin degree of freedom (spinons) in the lower bands can be obtained respectively as

\[ \xi^1(k) = \sqrt{U(\rho + E^1_X)} \hspace{1cm} (25) \]

and

\[ \xi^{(2)}(k) = E^{(2)}_f \hspace{1cm} (26) \]

Comparing equation (22) with equation (3), it is obvious that the structure of the energy spectrum \( \xi(k) \) of the spinon in the case of interacting is the same as the one of the non-interacting electron. The difference is that the model parameters \( t, \lambda \) and \( \alpha \) in the energy spectrum of the spinon are renormalized by the interactions. There are three definitions of these renormalized model parameters as follows

\[ t^R = Q_f t, \hspace{1cm} \lambda^R = Q_f \lambda, \hspace{1cm} \alpha^R = Q_f \alpha. \hspace{1cm} (27) \]

The similarity between the two spectra of spinons and non-interacting electron has important consequences for the Rashba SOC-driven topologically trivial and non-trivial transition that will be discussed later.

The definitions of five mean field parameters, i.e. equations (10)–(14) and the constraint equation of the X-field, i.e. \( |X|^2 = 1 \) are actually the six self-consistency equations in the slave-rotor mean field method. We obtain these self-consistency mean field equations as

\[ \frac{1}{2\Lambda} \sum_k \frac{\sqrt{U}}{2\sqrt{\rho + E^X_k}} + x_0 = 1, \hspace{1cm} (28) \]

\[ Q_f = \frac{1}{6\Lambda} \sum_k \frac{\text{sgn}(tQ_X - \alpha Q'_X)|g\sqrt{U}}{2\sqrt{\rho + E^X_k}} + x_0, \hspace{1cm} (29) \]

\[ Q'_f = \frac{1}{12\Lambda} \sum_k \gamma X \cdot \frac{\sqrt{U}}{2\sqrt{\rho + E^X_k}} + x_0, \hspace{1cm} (30) \]

\[ Q_X = \frac{1}{6\Lambda} \sum_k [(u^1_1 u^1_2 + u^1_3 u^1_4 + u^1_5 u^1_6)g + \text{c.c}] \hspace{1cm} (31) \]

\[ Q'_X = \frac{1}{12\Lambda} \sum_k [(u^1_1)^2 + (u^1_2)^2 + (u^1_3)^2 + (u^1_4)^2 - (u^1_5)^2 \gamma X, \hspace{1cm} (32) \]

\[ Q''_X = \frac{1}{6\Lambda} \sum_k [(u^1_5 - i u^1_6)(u^1_1 u^1_4 + u^1_2 u^1_3) + (u^1_5 + i u^1_6)(u^1_2 u^1_3 + u^1_4 u^1_6) + \text{c.c}. \] \hspace{1cm} (33) \]

Here \( u^1_1, u^1_2, \ldots, u^1_6 \) are the components of vectors \( u^1_1, u^1_3, u^1_6 \)

\[ u^1_1 = (u^1_1, u^1_2, u^1_3, u^1_4)^T \] 

and \( u^1_2 = (u^1_2, u^1_3, u^1_4, u^1_5)^T \) are the eigenvectors of the Hamiltonian matrix \( H^f \), corresponding to the two lower eigenenergies \( E^{(1)}_f \) and \( E^{(2)}_f \) respectively and can be obtained analytically or numerically by computer.

3.2. The Mott transition of the charge degree of freedom

In the slave-rotor mean field method, the gap of the charge degree of freedom is closed when the interaction \( U \) is small. The condensed charge combines the spinon to form the conventional physical electron. In the larger-\( U \) region, the gap
of the charge degree of freedom can be opened and a spin-charge separation occurs. There is a Mott transition of the charge degree of freedom. At the Mott transition, the condensate density of charges $x_0 = 0$ and $\rho = -\min(E^\alpha_{\text{topo}})$ derived from equation (25). Under the two conditions, we can solve numerically the six mean field self-consistency equations i.e. equations (28)–(33) and obtain the boundary of Mott transition as shown in figure 6.

From equations (3) and (22), the spinon has the same band structure as the one of conventional physical electron of the R–KM model which is topologically non-trivial in the case of small Rashba SOCs $\chi < \chi_{\text{topo}}$. Therefore, below the boundary of the Mott transition the combined phase may be a correlated $Z_2$ topological insulator which connects adiabatically to the one possessed by the R–KM model. It have been investigated that the Rashba SOC can drive the R–KM model into a topologically non-trivial SM or trivial metal state from $Z_2$ topological insulators. Therefore, the charge condensed phase may also be a topologically non-trivial SM or trivial metal state when the strength of the Rashba SOC beyond some critical values at which the indirect band gap of the spinon closes or the valence and conduction band can touch with each other. Above the boundary of the Mott transition, i.e. in the region of the charge uncondensed phase, it is a Mott insulator (MI) for the charge degree of freedom, while a QSL state for the spinon. There are also Rashba SOC-driven topologically trivial or non-trivial phase transitions of the spinon and novel quantum phases can emerge, as discussed below.

### 3.3. Influences of correlation on Rashba SOC-driven phase transitions in the region of charge condensed phase

As observed from equations (3) and (22), the energy band of the spinon with the renormalized electron hopping $t$, intrinsic SOC $\lambda$ and Rashba SOC $\alpha$ as defined in equation (27) has the same structure as the one of non-interacting electrons of R–KM model. In the model without strong correlations, topologically trivial and non-trivial transitions of electrons occur at $\alpha = \chi_{\text{topo}} \cdot \lambda$ and $\alpha = \chi_{\text{topo}} \cdot \lambda^R$ respectively. It is obvious that, for spinons, the topologically trivial or non-trivial transition can occur at $\alpha^R = \chi_{\text{topo}} \cdot \lambda^R$ or $\alpha^R = \chi_{\text{topo}} \cdot \lambda^R$. Moreover, the condensate density of charges $x_0 \neq 0$ at the point $(\imath \nu^0_n, k^0)$ and the gap of the charge degree of freedom is closed, i.e. $\rho = -\min(E^\alpha_{\text{topo}})$ when charges condense. Thus, we obtain the conditions

$$x_0 \neq 0, \quad \rho = -\min(E^\alpha_{\text{topo}}), \quad \alpha = \chi_{\text{topo}} \cdot \lambda \frac{Q_f}{Q_f}$$

(34)

for topologically trivial transition of spinons and

$$x_0 \neq 0, \quad \rho = -\min(E^\alpha_{\text{topo}}), \quad \alpha = \chi_{\text{topo}} \cdot \lambda \frac{Q_f}{Q_f}$$

(35)

for topologically non-trivial transition of spinons in the region of the charge condensed phase. The Rashba SOC-driven topologically trivial and non-trivial transition in the charge condensed phase can be obtained by solving numerically the self-consistency equations (28)–(33) under the conditions (34) and (35) respectively. The results are shown in figure 7. For $U = 0$, we reproduce the earlier result of non-interacting limit that is $\alpha = \chi_{\text{topo}} \cdot \lambda$ and $\alpha = \chi_{\text{topo}} \cdot \lambda$ for the topologically trivial and non-trivial transition respectively, because of $Q_f = 1$ and $Q_f = 1$ at $U = 0$. The behavior of $Q_f$ and $Q_f$ is shown in figure 8.

An important investigation that we want to make is the influence of strong correlations on the Rashba SOC-driven transition. From our numerical results, it can be seen that the critical $\alpha$ for both topologically trivial and non-trivial transition shifts to the smaller value with increasing $U$ for each $\lambda$. There is a narrow window where a TSM exists. It is similar to the case of non-interacting limit. For topologically trivial transition, the region of correlated $Z_2$ topological insulator is shrunk and the correlation destabilize the
correlated topological phase. The correlation has the similar behavior on the topologically non-trivial transition, i.e. it destabilizes the correlated TSM phase. As a consequence, the region of TSM phase shrinks slightly with the increasing correlation. Furthermore, the larger intrinsic SOC can lead to the wider region of TSM phase. For the small intrinsic SOC the region is very narrow, e.g. the case of $\lambda = 0.1$ as shown in figure 7(a).

In particular, when the phase boundary of spinon reaches the Mott boundary, the topologically trivial or non-trivial transition of spinons and the Mott transition of charge degree of freedom occur simultaneously. This can also be obtained from self-consistency equations under the condition as $x_0 = 0$, $\rho = -\min(E^0_\lambda)$ and $\alpha = \chi_{\text{topo}} \cdot \lambda \frac{\partial \rho}{\partial T}$, and the special transition points are marked out by black points in figures 6 and 7.

Along the topologically trivial or non-trivial phase boundary, the condensate density $x_0$ should decrease with the increasing correlation. The behavior of the condensate density is shown in figure 9. The condensate density has the maximum value at $x_0 = 1$ at $U = 0$ and is equal to zero when the boundary of topologically trivial transition of the spinon reaches the Mott boundary of the charge degree of freedom. In our numerical calculation, for each intrinsic SOC, the condensate density along the boundary of the topologically non-trivial transition shifts slightly compared to the one along the boundary of the topologically trivial transition. So we do not draw it here.

3.4. Influences of correlation on Rashba SOC-driven phase transitions in the charge Mott region

In the Mott region of the intermediate strength of correlations, there is no condensate of the charge degree of freedom, i.e. $x_0 = 0$ and the gap of charge degree of freedom is opened, i.e. $\rho \neq -\min(E^0_\lambda)$. The conditions that the topologically trivial and non-trivial transition occur in the Mott region of charge degree of freedom can be obtained respectively as

$$x_0 = 0, \quad \rho \neq -\min(E^0_\lambda), \quad \alpha = \chi_{\text{topo}} \cdot \lambda \frac{\partial \rho}{\partial T},$$

(36)

and

$$x_0 = 0, \quad \rho \neq -\min(E^0_\lambda), \quad \alpha = \chi_{\text{topo}} \cdot \lambda \frac{\partial \rho}{\partial T},$$

(37)

Under the condition (36) or (37) for the Rashba SOC-driven transition, the altered self-consistency equations are solvable. Boundaries of the topologically trivial and non-trivial transition in the Mott region of charge degree of freedom are shown in figure 11.

The influences of correlations on the Rashba SOC-driven topologically trivial or non-trivial transition in the charge Mott region are similar to the case of condensed charges. For topologically trivial transition, the correlation destabilizes the insulating phase of the spinon which possesses the same band structure as the $Z_2$ topological insulator in the region of condensed charges. Before the topologically trivial transition, the phase is a mixed state of the MI of charges and the QSL of spinons with the topologically non-trivial band structure, which is actually a TMI [30, 51]. After the topologically trivial transition, the indirect energy gap of spinons is closed and the mixed state becomes a TMI with gapless spin excitations (we call it TMI$^\star$). For the topologically non-trivial transition, the correlation also destabilizes the topologically non-trivial phase (TMI$^\star$). After this transition, the QSL component in the mixed phase becomes a topologically trivial state due to the band touching of valence and conduction bands of spinons, and maintains the gapless spin excitation.

To consider the stability of the QSLs or TMI and TMI$^\star$ associated with quantum fluctuations, our zeroth-order mean-field method should be extented to the first-order mean-field theory via the introduction of the $U(1)$ or $SU(2)$ gauge field coupled to the spinon [52]. To obtain a stable mean-field QSL or TMI ($\text{or TMI}^\star$), we should give gauge fluctuations a finite energy gap. Young et al [25] have supposed that when another coupled honeycomb lattice layer is added one can open up a gap for gauge field. This suppresses the gauge fluctuation, and then the QSLs or TMI and TMI$^\star$ are stable in this situation. So we are not concerned with quantum fluctuations and assume that these mean-field QSLs are stable in this work.

We can summarize above discussions to obtain the phase diagram of the R–KMH model as shown in figure 11. Phase boundaries in phase diagrams can be observed in detail from figures 6, 7 and 10. For the small intrinsic SOC (e.g. $\lambda =$
and the emergence of TMI or TMI∗ Rashba SOC-driven transitions of the spin degree of freedom. Our phase diagram reveals the influences of correlations on the effect of the strong correlation. In the region of the spinon, it is essential that the ratio $\chi$ possessed by the boundary of the Rashba SOC-driven topologically non-trivial transition is no longer equal to the well-known value $2\sqrt{3}$ and does decrease with the increasing intrinsic SOC. It is worth mentioning here that the boundary of the Rashba SOC-driven topologically non-trivial transition in the case of large intrinsic SOCs, even in the region of the physical electron, is obtained for the first time.

4. Conclusions and outlook

The competition between the Rashba SOC and the intrinsic SOC can lead to the rich phenomena. For the small intrinsic SOC, we investigate the effects of the Rashba SOC on the band structure of KM model when $\chi > \chi_{\text{topo}} = \chi_0$, where $\chi_0 = 2\sqrt{3}$ is the classical critical ratio at which the topologically non-trivial transition occurs. The Rashba SOC cannot open the gap, but maintains touching points at $K$ and $K'$ and adds three satellite touching point around the $K$ or $K'$. For the large intrinsic SOC, we find that the critical $\chi_{\text{topo}}$ at which topologically non-trivial transition or the band touching occurs decreases with the increasing intrinsic SOC due to the deformation of the band caused by the Rashba SOC. Furthermore, there are three touching points which are located around $K$ or $K'$. When $\chi_{\text{topo}} < \chi < \chi_0$, the three points are split into six touching points. The inside three points move toward the $K$ or $K'$ and eventually shrinks into a single point at $K$ or $K'$ when $\chi = \chi_0$. The phenomenon when $\chi > \chi_0$ is the same as the one when $\chi > \chi_{\text{topo}}$ in the case of small intrinsic SOCs. For all the intrinsic SOCs, the indirect gap has closed before the band touching occurs. This fact has been reported by others implies a Rashba SOC-driven topologically trivial transition. Including the topologically non-trivial transition, the two Rashba SOC-driven transitions lead to three distinct phases possessed by R–KM model, i.e. the $Z_2$ TI, the TSM phase and the metal phase. When the correlation is introduced, new phases can arise from these non-interacting phases.

Effects of the correlation are investigated by the slave-rotor mean field method. There is a Mott transition of charge degree of freedom and the band topology of the electron in the non-interacting model is inherited by the spinon. Below the Mott boundary, correlations can let the smaller Rashba SOC to drive the topologically trivial and non-trivial transition.

Figure 10. Boundaries of topologically trivial and non-trivial transitions of the spinon in the Mott region of the charge degree of freedom. (a) $\lambda = 0.1$, (b) $\lambda = 0.4$. The black points represent the special points on the boundaries of Mott transition at which the topological trivial or non-trivial transition occurs.

Figure 11. Phase diagrams of the R–KMH model at (a) $\lambda = 0.1$ and (b) $\lambda = 0.4$. The magnetically ordered phase at the larger $U$ have been discussed by Laubach et al [44]. The red dashed line in (b) corresponds to the $\chi_0 = 2\sqrt{3}$ and does not the boundary of topologically trivial or non-trivial transition at $\lambda = 0.4$. 
transition of physical electrons and destabilize correlated $Z_2$ TI and TSM phase. These results are qualitatively consistent with the one given by VCA in the case of small intrinsic SOC. Above the Mott transition, the correlation has the similar behavior on the two Rashba SOC-driven transition of spinons. Because of the uncondensed charge in the Mott region, the correlation destabilizes two topological mixed phases of the charge degree of freedom and the spinon (not the physical electron now), i.e. TMI and TMI*. The effects of correlations are summarized in phase diagrams of the R–KMH model (see figure (11)). In particular, for the large intrinsic SOC (e.g. $\lambda = 0.4$), the boundaries of the Rashba SOC-driven topologically non-trivial transition in both the charge condensate and Mott regions are obtained for the first time. These boundaries correspond to the ratio $\chi$ of the R–KM model which is not equal to the well-known value $2\sqrt{3}$ but decreases with the increasing intrinsic SOC.

The breaking of both mirror and hexagonal symmetries can lead to the anisotropic Rashba SOC, effects of which on the energy spectrum of the two-dimensional electron gas [53], metallic surface states [54] or electrons in graphene sheet [55] have been investigated. The spin polarization can be influenced by the anisotropic Rashba SOC and there is a Lifshitz transition. The effects of the anisotropy of the Rashba SOC may make the competition between the Rashba SOC and the intrinsic SOC more interesting. Furthermore, the correlation may also have important influences on the competition in the case of the anisotropic Rashba SOC.

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