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# Symmetry protection of quantum phase transitions in honeycomb lattice

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ABSTRACT

Based on an analytical model of topological insulator, we present the quantum phase transitions of topological insulators with different symmetries by calculating their phase diagrams and edgestates. In particular, we show the symmetry protection nature of the topological quantum phase transitions. Topological quantum phase transitions cannot be classified by symmetries. However, the symmetry of the system plays an important role, where different topological quantum phase transitions are protected by different global symmetries.



## 1. Introduction

Recent discovery of the two-dimensional (2D) and three-dimensional (3D) topological insulator (TI) states has generated great interests in this new state of topological quantum matter [1–7]. These insulators differ in subtle but essential ways from ordinary band insulators. For example, in the presence of a sample boundary, these insulators necessarily possess gapless edgestates inside the bulk energy gap. The existence of edge channels is due to the nontrivial topology of the bulk energy bands. The first topological invariant is called as Chern number or TKNN invariant [8,9] which measures the quantized Hall conductivity. There are two other nontrivial topological invariants that are proposed to describe this topology virtually at the same time: $Z_2$ invariant [10] proposed by Kane and Mele and spin-Chern number proposed by Sheng et al. [11]. It is well known that in Landau theory different orders are classified by symmetries [12]. The phase transitions of these orders, which occur when a driving parameter in the Hamiltonian of the system changes across a critical point, are always accompanied by the global symmetry breaking. However, there is also an exception that can only be witnessed by the topological invariants. Without closing the gap, energy spectra with different topologies cannot be deformed into each other. This is because a topological quantum phase transition occurs when changing the topological invariants.

Thus, an interesting issue is what a role symmetry [13,14] plays in topological insulators [16–20]. For a deeper understanding and quantitative predictions of novel phenomena associated with topological insulators, in the present work, we investigate transitions between phases of matter with topological order. Using both analytical models and numerical calculations we reveal the relationship between symmetry and phase transition. We find that with the increase of the Rashba-type term which keeps the time reversal symmetry (TRS) but breaks the $S_z$ symmetry the quantum spin Hall (QSH) state turns into a normal insulator (NI) state directly. While with the increase of the staggered magnetic term $M$ which breaks the TRS but keeps the $S_z$ symmetry the QSH state turns into the quantum anomalous Hall (QAH) state firstly before it goes into the NI state ultimately. Furthermore, we calculate the edgestates of these topological phases.

The rest of the paper is organized as follows. In Section 2, we introduce the 2D honeycomb lattice model. In Sections 3 and 4, we discuss the results for the system coupling with a Rashba-type spin orbital coupling and a staggered magnetic field, respectively. Based on the global phase diagram and the edgestates, we show the symmetry protection nature of the topological quantum phase transitions. Finally, we conclude this work with a general discussion of the relationships between symmetry and phase transition in Section 5.

## 2. Model analysis

We will start from a 2D honeycomb lattice model [21–23], and then couple it with a Rashba-type spin orbital coupling and a staggered magnetic field. The Hamiltonian of our model, which

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is relevant to the 2D electrons in a single-atomic layer graphene system, is given by the following form:

$$H = t\sum_{\langle i,j\rangle} c_i^\dagger c_j + it'\sum_{\langle\langle i,j\rangle\rangle} \nu_{i,j} c_i^\dagger s_z c_j + \lambda_\upsilon \sum_i \xi_i c_i^\dagger c_i + \lambda_R \sum_i c_i^\dagger (s_y \times \tau_y) c_i + M\sum_i \omega_i c_i^\dagger c_i, \tag{1}$$

where $i$ labels the sites of the honeycomb lattice, $c_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger)$ are the electron creation operators, and $s$ and $\tau$ are the Pauli matrices which are the identities for the spin and orbital indices, respectively. The first term is the nearest neighbor hopping term, where we have suppressed the spin index on the electron operators. The second term is the mirror symmetric spin orbit interaction which involves spin dependent second neighbor hopping. Here $\nu_{i,j} = \frac{2}{\sqrt{3}}(\hat{d}_1 \times \hat{d}_2)_z = \pm 1$, $i$ and $j$ are the two next-nearest neighbors, and $\hat{d}_1$ and $\hat{d}_2$ are the unit vectors along the two bonds. The third term is a staggered sublattice transition which is positive for A sublattice and negative for B sublattice ($\xi_i = \pm 1$). The fourth term is the Rashba-type spin orbital term which can be arised by a perpendicular electric field or interaction with a substrate. For simplicity, the Rashba-type term used here is in a relatively simple form. The fifth term is a phenomenological term which is used to describe the spin splitting induced by an external magnetic field or the magnetic doping [15]. The coefficient $\omega_i$ is positive for spin-up and negative for spin-down ($\omega_i = \pm 1$).

For the bulk honeycomb lattice, this Hamiltonian can be written in the momentum space. For each $k$ the Bloch wave function is a four-component eigenvector $|u(k)\rangle$ of the Bloch Hamiltonian matrix $H(k)$

$$H(k) = \Psi^\dagger \begin{pmatrix} \lambda_\upsilon + c + M & a - ib & 0 & -\lambda_R \\ a + ib & -\lambda_\upsilon - c - M & \lambda_R & 0 \\ 0 & \lambda_R & \lambda_\upsilon - c - M & a - ib \\ -\lambda_R & 0 & a + ib & -\lambda_\upsilon + c + M \end{pmatrix} \Psi. \tag{2}$$

Due to the two lattice degrees and two spin degrees, the Bloch wave function is a four-component eigenvector, shown as, $\Psi^\dagger = (\Psi_{A,\uparrow}^\dagger, \Psi_{B,\uparrow}^\dagger, \Psi_{A,\downarrow}^\dagger, \Psi_{B,\downarrow}^\dagger)$, $a = t(2\cos\frac{\sqrt{3}k_x}{2}\cos\frac{k_y}{2} + \cos k_y)$, $b = t(2\cos\frac{\sqrt{3}k_x}{2}\sin\frac{k_y}{2} - \sin k_y)$ and $c = 2t'(2\sin\frac{\sqrt{3}k_x}{2}\cos\frac{3k_y}{2} - \sin\sqrt{3}k_x)$. The Hamiltonian $H(k)$ gives four energy bands, of which two are occupied. As have been pointed out [10] that for $\lambda_R = M = 0$, there is an energy gap with magnitude $|3\sqrt{3}t' - \lambda_\upsilon|$. For $\lambda_\upsilon > 3\sqrt{3}t'$, the gap is dominated by $\lambda_\upsilon$, andthe system is a normal insulator. While $3\sqrt{3}t' > \lambda_\upsilon$ describes the QSH state. The staggered sublattice potential describes the transition between the QSH state and the NI state. From the expression of $a$, $b$ and $c$, we can see that without the Rashba-type term the system has $S_z$ symmetry but breaks the TRS. However, if the spin splitting term $M$ equals to zero, the system keeps TRS but breaks $S_z$ symmetry. In the following, we will divide into two parts to discuss the relationship between the global symmetry and the phase transition.

## 3. System with TRS but without $S_z$ symmetry

### 3.1. Global phase diagram

We are here focusing on the case of $M=0$ which means that the system keeps TRS while breaks $S_z$ symmetry. By diagonalizing the Hamiltonian $H(k)$, the eigenvalues of the honeycomb lattice can be obtained as

$$E_k = \pm\sqrt{a^2 + b^2 + m^2 + \lambda_\upsilon^2 + \lambda_R^2 \pm 2\sqrt{b^2\lambda_R^2 + m^2\lambda_R^2 + m^2\lambda_\upsilon^2}}. \tag{3}$$

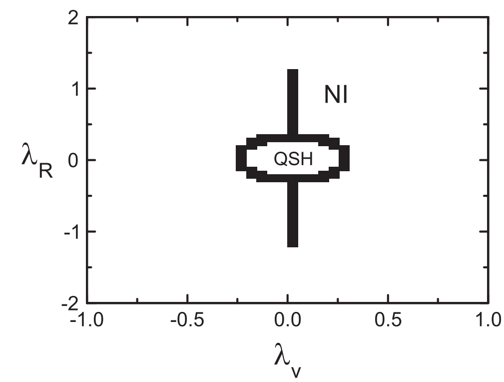


**Fig. 1.** The global phase diagram of the Hamiltonian with $M=0$. The parameters are $t=1$, $t'=0.1$.

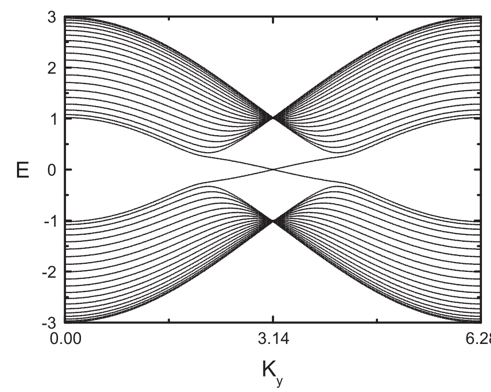


**Fig. 2.** The edgestate of the Hamiltonian without the magnetic term. The energy bands of spin-up and spin-down are doubly degenerate and the units of $E_k$ and $k_y$ are eV and $Å^{-1}$, respectively. The parameter is set to be $t=1$, $t'=0.05$, $\lambda_v=0$, the primitive vectors $a=\sqrt{3}$.

The parameters are that $t$ is set to be unit throughout this paper and $t'=0.1$. As mentioned above, the system is in the QSH state for $3\sqrt{3}t' > \lambda_\upsilon$ when $\lambda_R = 0$. We calculate the phase boundary by $E_k = 0$. Using the expression of $a$, $b$ and $c$, we obtain the global phase diagram with respect to $\lambda_R$ and $\lambda_\upsilon$ which is shown in Fig. 1. It can be seen that there are two phases in the global phase diagram, one is in the QSH state which is surrounded by the solid line and the others is in the NI state.

### 3.2. Edgestates

A more direct way of identifying the QSH phase is to study the edgestate spectrum. There are always an odd number of Kramers's pairs of edgestates on the boundary of a QSH insulator, and an even number pairs (possibly zero) for the boundary of a NI. To explore the edge topological invariant characterizing the QSH state, we now turn to study the honeycomb lattice ribbon with zigzag edges, That is, with periodic boundary condition in the $y$-direction and open boundary condition in the $x$-direction. Note that with this choice $k_y$ is still a good quantum number. By defining the partial Fourier transformation

$$c_{k_y}(x) = \frac{1}{\sqrt{L_y}}\sum_y c(x,y)e^{ik_y y}, \tag{4}$$

with $(x, y)$ as the coordinates of honeycomb lattice sites, the Hamiltonian can be rewritten. In this way, the 2D system can be treated as $L_y$ independent 1D tight-binding chains, where $L_y$ is the period of the lattice in the $y$-direction. The eigenvalues of the 1D Hamiltonian $H(k_y)$ can be obtained numerically for each $k_y$, as shown in Fig. 2. An important property of the spectrum is the