Topological States in Two-Dimensional Su-Schrieffer-Heeger Models

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(Dated: August 9, 2022)

We study the topological properties of the generalized two-dimensional (2D) Su-Schrieffer-Heeger (SSH) models. We show that a pair of Dirac points appear in the Brillouin zone (BZ), consisting a semimetallic phase. Interestingly, the locations of these Dirac points are not pinned to any high-symmetry points of the BZ but tunable by model parameters. Moreover, the merging of two Dirac points undergoes a novel topological phase transition, which leads to either a weak topological insulator or a nodal-line metallic phase. We demonstrate these properties by constructing two specific models, which we referred as type-I and type-II 2D SSH models. The feasible experimental platforms to realize our models are also discussed.

I. INTRODUCTION

Topological phases of matter have attracted tremendous research interests in recent decades [1, 2]. Among those famous topological models, the 1D Su-Schrieffer-Heeger (SSH) model provides a prototype and simple model endowed with rich physics to investigate topological phenomena in condensed matter physics [3]. It exhibits fascinating topological properties such as the topological phase transitions associated with Zak phase and fractional fermions number at the ends of the sample [3]. It also helps to clarify the theory of bulk polarization based on Berry phase [4], which has wide and deep impacts on condensed matter physics in recent decades, especially on the development of topological band insulators [5, 6].

Recently, the 1D SSH model has been extended to 2D on a square lattice. For instance, Liu et al. found that the 2D SSH model shows nontrivial topological phases even the Berry curvature is zero in the whole BZ [7]. Benalcazar et al. extended the 1D SSH model to two-, and three-dimensional systems with a $\pi$-flux inserted at each plaquette of the lattice. The proposed Benalcazar-Bernevig-Hughes (BBH) models hold quantized bulk quadrupole and octupole moments in 2D and 3D, respectively [8, 9]. Similar to 1D SSH model, bound states carrying fractional charges exist at the corners of the system. Thus the BBH provides a concert example for the higher-order topological insulators (HOTIs). Such HOTIs generalize the conventional bulk-boundary correspondence. Typically, a topological bulk state in $d$-dimension has robust $(d - 1)$-dimensional boundary states. Nevertheless, HOTIs have localized states at boundaries that are two or three dimensions lower than the bulk. The HOTIs have consequently attracted both theoretical and experimental interest over past years [10–31], and the higher-order topological protection has been extended to superconductors [32–38] and semimetals [39–41].

Since several types of 2D SSH models are possible when generalizing the 1D SSH model, it is thus natural to ask whether these models exhibit interesting topological properties. In this work, we investigate the properties of two typical kinds of 2D SSH models. Remarkably, we find that these models have rich topological phases. In the semimetallic phase, a pair of Dirac points appear in the BZ. Interestingly, the locations of the Dirac points are not pinned but can be easily tuned by continuous parameter modulations without breaking any symmetries. The merging of two Dirac points will experience a novel topological phase transition which transform the system to either a weak topological insulator or a nodal-line metallic phase. We demonstrate the topological properties of these different phases by employing two independent winding numbers together with boundary signatures and symmetry arguments. We also discuss how to realize our model experimentally based on synthetic quantum materials.

The remainder of this paper is organized as follows. Section II introduces the type-I 2D SSH model and its band structure. Section III presents the semimetallic phases of the type-I 2D SSH model. Section IV shows the anisotropic nature of type-I 2D SSH model. Section V considers properties of type-II 2D SSH model. Finally, we conclude our results with a discussion in Section VI.

II. TYPE-I TWO-DIMENSIONAL SSH MODEL

Let us focus on the type-I 2D SSH model first [42]. We consider a type-I 2D SSH model as shown in Fig. 1(a), where the weak (thin) bonds and strong (thick) bonds are alternately dimerized along the two adjacent parallel lattice rows (x-direction) or columns (y-direction). The four orbital degrees of freedom in each unit cell are labeled as $1 - 4$. For clarity, we consider spinless fermions.
The lattice Hamiltonian is
\[ H_1 = \sum_\mathbf{R} \left( t_x C^\dagger_{\mathbf{R},3} C_{\mathbf{R},3} + t C^\dagger_{\mathbf{R},2} C_{\mathbf{R},4} + h.c. \right) + \sum_\mathbf{R} \left( t_b C^\dagger_{\mathbf{R},2} C_{\mathbf{R},3} + t C^\dagger_{\mathbf{R}} C_{\mathbf{R},4} + h.c. \right) + \sum_\mathbf{R} \left( t C^\dagger_{\mathbf{R},1} C_{\mathbf{R}+\ell,3} + t C^\dagger_{\mathbf{R}+\ell,1} C_{\mathbf{R},3} + h.c. \right) + \sum_\mathbf{R} \left( t y C^\dagger_{\mathbf{R}} C_{\mathbf{R}+\ell,4} + t C^\dagger_{\mathbf{R}+\ell,2} C_{\mathbf{R},4} + h.c. \right), \tag{1} \]

where \( C^\dagger_{\mathbf{R},i} \) is the creation operator for the degree of freedom \( i \) in the unit cell \( \mathbf{R} \) with \( i = 1, 2, 3, 4 \), as shown in the Fig. 1(a). Transforming it into the reciprocal space, the effective Bloch Hamiltonian describing the type-I 2D SSH model reads

\[ H_1(\mathbf{k}) = \begin{pmatrix} 0 & q_1(\mathbf{k}) \\ q_1^*(\mathbf{k}) & 0 \end{pmatrix}, \tag{2} \]

\[ q_1(\mathbf{k}) \equiv \left( \begin{array}{cc} t_x + t e^{i k_x} & t + t y e^{i k_y} \\ t_y + t e^{-i k_x} & t + t x e^{-i k_y} \end{array} \right); \tag{3} \]

where \( \mathbf{k} = (k_x, k_y) \) is the 2D wave-vector; \( t \) and \( t_{x/y} \) are the staggered hopping amplitudes along \( x/y \)-directions. For simplicity, we put the lattice constant to be unity and assume \( t > 0 \) hereafter. From its off-diagonal form, the Hamiltonian in Eq. (2) respects chiral (sublattice) symmetry. Explicitly, the chiral symmetry is \( C H(\mathbf{k}) C^{-1} = -H(\mathbf{k}) \) with the chiral-symmetry operator \( C = \tau_3 \otimes \sigma_0 \), where \( \tau \) and \( \sigma \) are Pauli matrices for different orbital degrees of freedom in the unit cell. The energy bands and corresponding wave functions can be obtained analytically. The energy bands of Eq. (2)

\[ E^\pm_q(\mathbf{k}) = \pm \sqrt{\xi_q^2(\mathbf{k}) + \zeta_q^2(\mathbf{k})} = \pm |\varepsilon_q(\mathbf{k})|, \tag{4} \]

where we have defined \( \xi_q(\mathbf{k}) \equiv (t + t_x) \cos \frac{k_x}{2} + \eta(t + t_y) \cos \frac{k_y}{2}, \zeta_q(\mathbf{k}) \equiv (t - t_x) \sin \frac{k_x}{2} - \eta(t - t_y) \sin \frac{k_y}{2}, \) and \( \varepsilon_q(\mathbf{k}) \equiv \xi_q(\mathbf{k}) + i \zeta_q(\mathbf{k}) \) with \( \eta = \pm 1 \). The convenient form of energy bands Eq. (4) will help us to locate the Dirac points and identify the phase diagram of the system.

III. SEMIMETALLIC PHASES

The type-I 2D SSH model actually possesses three different topological phases, as shown in the phase diagram Fig. 1(b). Here we first discuss the semimetallic phase with a pair of Dirac points within the region \( |t_x + t_y| < 2t \) and \( t_x \neq t_y \). Due to the presence of chiral symmetry, the conduction and valence bands touch at zero energy [Fig. 2(a)]. Thus, the existence of Dirac points is constrained by the conditions \( \xi_q(\mathbf{k}) = \zeta_q(\mathbf{k}) = 0 \). Consequently, we find a pair of Dirac points located at \( \mathbf{K}_\pm \equiv \pm (K_x, -K_y) \), where \( K_{x/y} \) are given by

\[ K_{x/y} = 2 \arccos \frac{(t + t_{y/x})^2 (2t - t_x - t_y)}{4t^2(t - t_x t_y)}. \tag{5} \]

Astonishingly, the Dirac points are not pinned to any high-symmetry points but are highly tunable by parameter modulations. If we consider a simple parameterization with \( t_x = s \in [0, t], t_y = t - s, \) and \( t = 1 \), we find that the relation \( K_x + K_y = 2t/3 \) holds true. As a result, the Dirac points move along a line segment when we vary the parameter \( s \). Interestingly, no symmetries are broken as we move around Dirac points by variation of \( t_x \) and \( t_y \). The Dirac points are topologically protected by a quantized charge \( Q_{\mathbf{K}_\pm} = \frac{1}{2\pi} \oint \mathbf{dk} \cdot \mathbf{\nabla} [q^{-1}(\mathbf{k}) \mathbf{\nabla} q(\mathbf{k})] \), where the loop \( \ell \) is chosen such that it encircles a single Dirac point \( \mathbf{K}_\pm \). In essence, it is based on the \( \pi \) Berry phase, which is actually the same as in graphene. The two Dirac points in the BZ have opposite topological charges \( Q_{\mathbf{K}_\pm} = \pm 1 \). They annihilate each other when they meet in \( k \)-space.

Let us then turn to the nodal-line metallic phase under the specific condition \( t_x = t_y \) [Fig. 2(b)]. From Eq. (4), we find that the system exhibits a gapless nodal line at

\[ k_x + k_y = 0, \text{ if } t_x = t_y \neq t. \tag{6} \]

The appearance of a gapless nodal line is a direct consequence of accidental mirror symmetry along the line \( x + y = 0 \). In momentum space, the mirror symmetry is expressed as \( MH(k_x, k_y) M^{-1} = H(-k_y, -k_x) \). Note that the Hamiltonian \( H(\mathbf{k}) \) commutes with the mirror operator \( M \) along the nodal-line \( k_x + k_y = 0 \). Therefore, we can label the eigen states of the Hamiltonian \( H(\mathbf{k}) \) by the eigen states of mirror operator \( M \) as

\[ H(\mathbf{k}) |\pm\rangle = \pm E |\pm\rangle, M |\pm\rangle = |\pm\rangle. \tag{7} \]
We further note that the mirror operator commute with the chiral symmetry operator, i.e., $[C, M] = 0$. Therefore, we can show that $C|+$ is also an eigenstate of $M$ with eigen value $+1$. Moreover, $C|+$ is eigenstate of $H(k)$ with energy $+E$. Actually, the chiral symmetry maps the state $|+$ with energy $+E$ to state $C|+$ with energy $-E$. This implies that those states are degenerated states at energy $E = 0$.

IV. WEAK TOPOLOGICAL INSULATING PHASES

The merging of two Dirac points can transfer the system from the semimetallic phase to a weak topological insulator, which provides a novel type of topological phase transition. Figure 2(c) presents the band structure at the critical merging points, at which the spectrum stays linear along one direction while becomes parabolic along another direction [45]. Specifically, the weak topological insulators is located in the region $|t_x + t_y| > 2t$ and $t_x \neq t_y$. The weak topological insulators possess a direct band gap, see Fig. 2(d). It is described by two winding numbers $(w_x, w_y)$ with one of them being one and the other being zero. The winding number is defined as

$$w_{x/y} = \frac{1}{2\pi i} \int_0^{2\pi} dk_{x/y} \text{Tr}[q_1^{-1}(k)] \partial k_{x/y} q_1(k)$$

for arbitrary $k_{y/x} \in [0, 2\pi]$. Actually, this weak topological insulators can be further divided into two subphases: (i) $w_x = 1, w_y = 0$ ($t_x > t_y$ and $|t_x + t_y| > 2t$) and (ii) $w_x = 0, w_y = 1$ ($t_x < t_y$ and $|t_x + t_y| > 2t$). When $w_x = 1, w_y = 0$ ($w_x = 0, w_y = 1$), the system is nontrivial along $x(y)$-direction and trivial along $y(x)$-direction. It is clear that once crossing the boundary $t_x = t_y$ the system will shift from subphase (i) to subphase (ii) or vice versa. Correspondingly, a totally flat edge band exists in the gap of the energy spectrum of a ribbon along $x(y)$-direction for the subphase (i) (subphase (ii)). Figures 3(a) and (b) present the band structure of a ribbons along $x$- and $y$-direction, respectively, for the subphase (ii). The flat edge bands exist only in Fig. 3(a). Notably, neither the topologically trivial insulator with $w_x = w_y = 0$ nor the nontrivial phase with $w_x = w_y = 1$ appear in the inclined 2D SSH model.

Furthermore, the calculation of Wannier bands can also provide consistent results with that of $w_{x/y}$ to identify the topological properties. Specifically, the Wilson loop operator parallel to $y$ direction is constructed as [38, 46]

$$\hat{P}_{y,k} = P_{N_y \delta k_y + k_y} P_{(N_y - 1) \delta k_y + k_y} \cdots P_{\delta k_y + k_y} P_{k_y},$$

where each projection operator is defined as $P_{m \delta k_y + k_y} \equiv \sum_{n \in N_{\text{occ}}} |n_{k_x, m \delta k_y + k_y}\rangle \langle u_{k_x, m \delta k_y + k_y}|$ with $|u_{k_x, m \delta k_y + k_y}\rangle$
with Dirac points here. The effective Bloch Hamiltonian describing the type-II 2D SSH model has the same form as Eq. (2) but with the off-diagonal parts replaced as

$$q_2(k) \equiv \begin{pmatrix} t_x + te^{ik_x} & t + te^{ik_y} \\ t_y + te^{-ik_y} & t_x + te^{-ik_x} \end{pmatrix}. \tag{10}$$

Its energy bands are

$$E_{\eta}^\pm(k) = \pm \sqrt{h_0(k) + \eta \sum_{j=x,y,z} h_j^2(k)}, \tag{11}$$

where we have defined the functions as $h_0(k) \equiv (t - t_x)^2 + 4t_y t \cos^2 \frac{k_y}{2} + (t^2 + t_y^2) \cos^2 \frac{k_y}{2}$, $h_x(k) \equiv 2 \cos \frac{k_y}{2} \left[ t(t_x + t_y) \cos(k_x + k_y/2) + (t^2 + t_x t_y) \cos \frac{k_y}{2} \right]$, $h_y(k) \equiv 2 \cos \frac{k_y}{2} \left[ t(t_x + t_y) \sin(k_x + k_y/2) + (t^2 + t_x t_y) \sin \frac{k_y}{2} \right]$, and $h_z(k) \equiv 2(t^2 - t_y^2) \cos \frac{k_y}{2}$. The type-II model has a glide-mirror symmetry: performing a mirror symmetry $M_x$ and then a half translation $g_y$ along $y$-direction, the system goes back to itself. Its Dirac points are located along $k_x = 0$ (or $k_x = \pi$) when $t_y > 0$ (or $t_y < 0$) [see Fig. 4(b)]. Explicitly, the Dirac points locate at $(0, \pm 2 \arccos \sqrt{\frac{(t_x + t_y)^2}{4t_y}})$ for $t_y > 0$ or $(\pi, \pm 2 \arccos \sqrt{\frac{(t_x - t_y)^2}{4t_y}})$ for $t_y < 0$. Corresponding, the physical solutions hold under the condition $(t + t_x)^2 < 4t_y t$ or $(t - t_x)^2 < -4t_y t$. The effective Hamiltonian close to the Dirac points can also be obtained analytically. For simplicity, let us focus on the case of $t_y > 0$. To this end, we need to get the two zero-energy eigen states at the Dirac points as a basis and then project the full Hamiltonian to the basis. Finally, the effective Hamiltonian is expressed as

$$H_{\text{eff}}(k) = v_x k_x \sigma_x - v_y k_y \sigma_y, \tag{12}$$

where $v_x = \sqrt{\frac{\sqrt{t(t-t_x)} + \sqrt{t(t+t_x)}}{t+|t_y|}}$, and $v_y = \text{sgn}(t+|t_y|) \sqrt{\frac{\sqrt{t(t-t_x)} + \sqrt{t(t+t_x)}}{t+|t_y|}}$.

V. TYPE-II TWO-DIMENSIONAL SSH MODEL

Now, let us consider another similar model: the type-II 2D SSH model, in which the alternatively dimerization pattern is shown in Fig. 3(a). The lattice Hamiltonian reads as

$$H_2 = \sum_R \left(t_x C_{R,1}^\dagger C_{R,3} + t_y C_{R,2}^\dagger C_{R,4} + \text{h.c.} \right)$$
+ \sum_R \left(t_x C_{R,1}^\dagger C_{R,4} + t_y C_{R,2}^\dagger C_{R,3} + \text{h.c.} \right)$$
+ \sum_R \left(t_x C_{R,1}^\dagger C_{R+\hat{x},3} + t_y C_{R,2}^\dagger C_{R+\hat{x},2} + \text{h.c.} \right)$$
+ \sum_R \left(t_x C_{R,1}^\dagger C_{R+\hat{y},4} + t_y C_{R,2}^\dagger C_{R+\hat{y},2} + \text{h.c.} \right). \tag{9}$$

The type-II model has many similarities with the type-I model, thus we just focus on the semimetallic phase
each unit cell and the alternately dimerized couplings between neighbours can be modulated the diameters that the sound wave go through. Another feasible platform to realize our model is based on ultracold gases in optical lattices \cite{52,53}, in which the lattice geometry and hopping strengths are adjustable.

Note that our results are distinctively different from recent reports to realize Dirac states in square lattices \cite{54,55}. These proposals require necessary \( \pi \) fluxes on each plaquette, and the Dirac points are pinned to boundaries of the BZ, which may makes it more difficult to detect experimentally. While our 2D SSH model does not require delicate manipulations of external flux. Interestingly, our models even provide platforms to realize the so called toric-code insulator \cite{56}.

In conclusion, we have proposed the 2D SSH models on a square lattice to realize tunable Dirac states. We have found that the locations of Dirac points are not pinned in the BZ but movable by parameter modifications. The merging of two Dirac points leads to a topological phase transition, which converts the system from a semimetallic state to a nodal-line metallic or a weak topological insulator. Our models even provide platforms to realize the so called toric-code insulator \cite{56}.

VII. ACKNOWLEDGMENTS

The author acknowledges S. B. Zhang, S. J. Choi, B. Fu, and B. Trauzettel for helpful discussions. This work was supported by the DFG (SPP1666 and SFB1170 “ToCoTronics”), the Würzburg-Dresden Cluster of Excellence ct.qmat, EXC2147, Project-id 390858490, and the Elitenetzwerk Bayern Graduate School on “Topological Insulators and topological superconductors” and the NSF of Zhejiang under Grant No. LQ20A04005.

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