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# The Zak phase and Winding number


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Bulk-edge correspondence is one of the most distinct properties of topological insulators. In particular, the 1-d winding number $\nu$ has a one-to-one correspondence to the number of edge states in a chain of topological insulators with boundaries. By properly choosing the unit cells, we show explicitly in the so-called extended SSH model that the winding numbers corresponding to the left and right unit cells may be used to predict the numbers of edge states on the two boundaries in a finite chain. Moreover, by modifying the definition of the Zak phase $\gamma$ to be summing over all the bands of the system, we show for a general two-band model that the modified Zak phase obeys $\gamma = 2\pi\nu$. It is thus always quantized even if there is no chiral symmetry in the system so that it is classified as trivial in the so-called periodic table of topological materials. We also carry out numerical calculation to demonstrate explicitly that the bulk-edge correspondence may indeed be generalized to this kind of systems.



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## I. Introduction

Since their discovery, topological materials have drawn a lot of attention in the community of condensed matter physicists[1]. Bulk-edge correspondence is one of the most distinct properties of topological insulators. In particular, the 1-d winding number $\nu$ has a one-to-one correspondence to the number of edge states in a chain of topological insulators with boundaries. When there is only a single connected boundary between the topological material and the environment, it is quite straight forward to make sense of the correspondence. On the other hand, if there are two or more disconnected boundaries, then it is sometimes not so easy to correctly interpret the results if we look into the details. For simplicity, let's consider a finite chain of the SSH model, which is one of the simplest topological materials[2, 3]. The number of edge states depends on whether the total number of sites in the system is even or odd. If the chain is in the topological phase and the number of sites is even, then there will be two edge states, which seems plausible since there are two boundaries after all. However, if the number of sites is odd, then there is always one edge state, which appears on either the left or right boundary depending on whether the inter-cell hopping amplitude is larger or smaller than the intra-cell hopping amplitude. Hence, it is not so straight forward to understand why this is the case.

Another awkward point regarding the 1-d topological materials is the Zak phase[4]. It is basically similar to the Berry phase and is believed to be somehow related to the topological nature of the system[5]. Each band of the system may give rise to an individual Zak phase. It is a general practice in the literature that the total Zak phase only includes those that their corresponding energy bands lie below the Fermi surface[6]. In particular, as far as a two-band model is concerned, only the Zak phase of the lower band is taken into account. Although it is indeed quantized when there is chiral symmetry in the system, it is generally not so if there is no chiral symmetry. There are two problems in our current understanding of the Zak phase. First of all, the topological nature of a system should be an intrinsic property of the whole system. Therefore, all the bands should have a say in determining which phase the system is in. Secondly, if the Zak phase is not always quantized, how can we use it to describe the topological property of a system?

In this paper, we try to address the above two problems. After some careful analysis, we put forward some possible resolutions. The rest of the paper is organized in the following way. In Sec. II, we first use the SSH model to carry out a detailed analysis of the bulk-edge correspondence. In a finite chain of SSH model, there are generally two boundaries, the left and right ones. To make the bulk-edge correspondence work sensibly, it is shown that we must choose the unit cells in such a way that they are consistent with the left and right boundaries. The winding numbers $\nu$ corresponding to the two unit cells may then be used to predict the numbers of edge states on the left and right boundaries. Then, we show that the bulk-edge correspondence would also work in the extended SSH model in which there are also next to nearest neighbor hopping amplitudes so that the highest winding number becomes 2. Of course, the results may be generalized to systems with even higher winding numbers. In Sec. III, we propose to modify the definition of the Zak phase $\gamma$ to be summing over all the bands. We show for a general two-band model that the modified


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Zak phase $\gamma = 2\pi\nu$ and thus is always quantized even if there is no chiral symmetry in the system contrary to naive expectation. We suspect there exists some yet to be identified crystalline symmetry in the system. Finally, we make conclusion and discuss possible extensions in Sec. IV.

## II. The winding number and the bulk-edge correspondence

Let's begin with the well-known SSH model, whose Hamiltonian is given by

$$H_{\mathrm{SSH}} = \sum_{j=-\infty}^{\infty} \left\{ \left( t_0 A_j^\dagger + t_1 A_{j+1}^\dagger \right) B_j \right\} + \text{h.c.}. \tag{1}$$

Here, $j$ denotes the unit cell, and $t_0, t_1$ are the intra-cell and inter-cell hopping amplitudes, respectively. Without loss of generality, we will assume $t_0, t_1$ to be both positive through out the paper for convenience. The Bloch Hamiltonian takes the following form

$$\mathcal{H}_{\mathrm{SSH}} = \begin{pmatrix} 0 & \bar{h}(k) \\ h(k) & 0 \end{pmatrix}, \tag{2}$$

with $h(k) = t_0 + t_1 \mathrm{e}^{ik}$. In terms of the Pauli matrices $\tau_i$'s, we have:

$$\mathcal{H}_{\mathrm{SSH}} = (t_0 + t_1 \cos k)\, \tau_1 + (t_1 \sin k)\, \tau_2. \tag{3}$$

It is obvious that the chiral operator $\Pi = \tau_3$ anti-commutes with $\mathcal{H}_{\mathrm{SSH}}$, which means that eigenstates of $\mathcal{H}_{\mathrm{SSH}}$ with non-zero energy always appear in pairs with eigenvalues $(E, -E)$ and the corresponding eigenstates are related by $|-E\rangle = \tau_3 |E\rangle$. In contrast, zero energy eigenstates can always be chosen to be chiral eigenstates and the left-handed and right-handed states are decoupled from each other.

Whether the system is in the topological phase or not may be determined by the 1-d winding number $\nu$ derived from $h(k)$, which traces out a closed contour in the complex plane as $k$ ranges over the Brillouin zone. It is well-known that the analytical expression for $\nu$ is given by

$$\nu = \frac{-i}{2\pi} \int_0^{2\pi} dk \frac{h'(k)}{h(k)}. \tag{4}$$

When $t_1 > t_0$, the contour will encircle the origin once so that $\nu = 1$, and the system is in the topological phase. In contrast, when $t_1 < t_0$, the origin will not be enclosed by the contour so that $\nu = 0$, and the system is in the trivial phase. According the so-called "bulk-edge correspondence", the most salient signature for a system being in the topological phase is the appearance of zero energy edge states on the boundaries of the system. However, it is also well-known that there is a freedom in choosing the unit-cell in the SSH model. Rather than grouping $A_j$ and $B_j$ to be the $j$-th unit-cell, we may rename $B_j$ and $A_{j+1}$ to be $\tilde{A}_j$ and $\tilde{B}_j$ for example and group them into a unit-cell instead. It is obvious that when we do this, the role of $t_0$ and $t_1$ will be interchanged and a system that is classified to be topological would become trivial under the new choice of unit-cell and vice versa. Naturally this leads to the question that if there is an ambiguity in determining whether a system is in the topological phase or not, then how we would be able to make sense of the bulk-edge correspondence? In order to resolve this difficulty, let's first consider a right semi-infinite SSH model so that there is an edge in the system:

$$H^{\mathrm{R}}_{\mathrm{SSH}} = \sum_{j=1}^{\infty} \left\{ \left( t_0 A_j^\dagger + t_1 A_{j+1}^\dagger \right) B_j \right\} + \text{h.c.}. \tag{5}$$

The energy eigenstates would satisfy the following recurrence relation and boundary condition:

$$\begin{aligned} &E A_j - (t_0 B_j + t_1 B_{j-1}) = 0; \\ &E B_j - (t_0 A_j + t_1 A_{j+1}) = 0, \\ &B_0 = 0. \end{aligned} \tag{6}$$

An edge state would be described by

$$A_j = \alpha s^j, B_j = \beta s^j. \tag{7}$$

By substituting the above expression into eq. (6), it reduces to

$$\begin{aligned} &E\alpha - \left(t_0 + t_1 s^{-1}\right) \beta = 0; \\ &E\beta - (t_0 + t_1 s)\, \alpha = 0; \\ &\beta = 0. \end{aligned} \tag{8}$$

To be consistent with the boundary condition, we see from the above equation that a non-trivial solution exists only if

$$E = 0, \text{and } s = -t_0/t_1. \tag{9}$$

For the wave function to be normalizable, we must have $|s| < 1$. This implies $t_1 > t_0$ and

$$A_j = A_1 \left(-t_0/t_1\right)^{j-1}, \; B_j = 0, \text{with } j \geq 1. \tag{10}$$

This is in accordance with the bulk-edge correspondence if we choose to group $A_j$ and $B_j$ into a unit-cell, which is certainly a natural thing to do in light of the system's boundary.

On the other hand, when we consider the left semi-infinite case so that

$$H^{\mathrm{L}}_{\mathrm{SSH}} = \sum_{j=-\infty}^{-1} \left\{ \left( t_0 A_j^\dagger + t_1 A_{j+1}^\dagger \right) B_j \right\} + \text{h.c.}. \tag{11}$$

The zero energy edge state would satisfy the same recurrence relation and boundary condition as in eq. (6).

However, a non-trivial solution now exists only if $t_1 < t_0$ and $A_{-j} = A_0 \left(-t_1/t_0\right)^j$, with $j \geq 0$. The result again may be made to be consistent with the bulk-edge correspondence if we now choose to group $B_j$ and $A_{j+1}$ into a unit-cell. To sum up, the bulk-edge correspondence would work out perfectly if we choose the unit-cell properly according to the boundary of the system.

We may make further check on this conclusion by considering a finite chain of the SSH model (see Fig. 1). Let's first consider the case that there are even number of sites:

$$H_{\text{SSH}}^{\text{even}} = \sum_{j=1}^{N-1} \left\{ \left( t_0 A_j^\dagger + t_1 A_{j+1}^\dagger \right) B_j \right\} + t_0 A_N^\dagger B_N + \text{h.c.}. \tag{12}$$

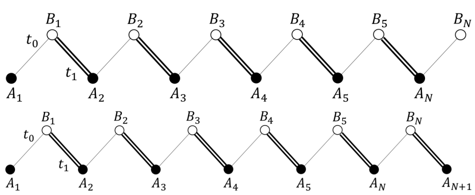



FIG. 1: The SSH system with $2N$ and $2N+1$ particles.

Using the standard technique to solve the recurrence relation, one finds that

$$\begin{aligned} &E = \pm\sqrt{t_0^2 + t_1^2 + t_0 t_1 \left(s + s^{-1}\right)}; \\ &t_0 \left( \frac{s^{N+1} - s^{-N-1}}{s - s^{-1}} \right) + t_1 \left( \frac{s^N - s^{-N}}{s - s^{-1}} \right) = 0. \end{aligned} \tag{13}$$

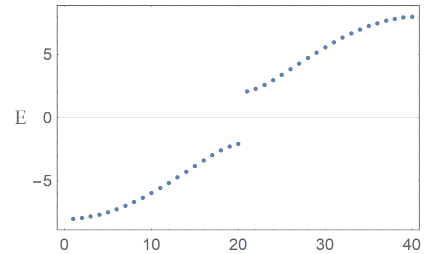
In this case, the solutions can only be found numerically. Because of the existence of the left and right boundaries, it is again natural for us to group $A_j$ and $B_j$ into a unit-cell. Based on the experience obtained in the right and left semi-infinite chains, we expect that edge states would exist only if $t_1 > t_0$. Since the left and right edges are now separated by a finite distance, there would be mixing between the two edge states. Consequently, the energy of these edge states would be approximately zero and the corresponding $s \approx -t_0/t_1, -t_1/t_0$. This indeed may be explicitly verified by numerical calculation, which is shown in Fig. 2. Therefore, it is in perfect agreement with the bulk-edge correspondence.

On the other hand, when there are odd number of sites in the system, we have

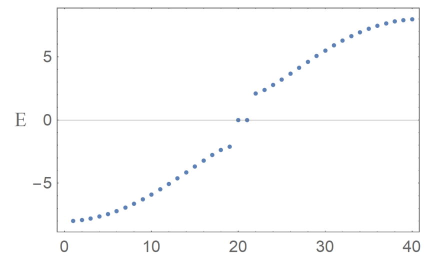
$$H_{\text{SSH}}^{\text{odd}} = \sum_{j=1}^{N} \left\{ \left( t_0 A_j^\dagger + t_1 A_{j+1}^\dagger \right) B_j \right\} + \text{h.c.}. \tag{14}$$

In this case, the recursion relation may be solved analytically:

$$s = e^{i\pi k/N}, \tag{15}$$




(a)

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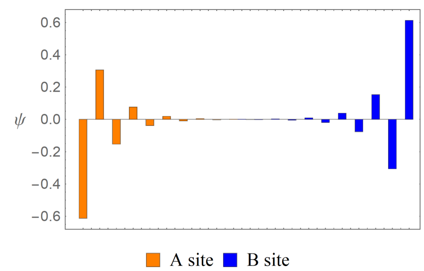
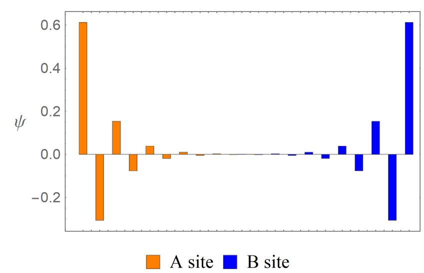



(c)




(d)

FIG. 2: (a) Energy spectrum in the trivial phase with $(t_0, t_1, N) = (5, 3, 20)$. (b) Energy spectrum in the topological phase with $(t_0, t_1, N) = (3, 5, 20)$. (c),(d) The wave function of the almost zero energy states in the topological phase.

with $k = 1, \ldots, N$, and

$$E_k = \pm\sqrt{t_0^2 + t_1^2 + 2t_0 t_1 \cos\left[\pi k/(N+1)\right]}. \tag{16}$$

In addition to the above $N$ pairs of energy eigenstates, there is also always an edge state with exact zero energy and $s = -t_0/t_1$ dictated by the chiral symmetry of the system. Note that when the total number of sites is odd, the unit-cell consistent with the left boundary is always different from the one that is consistent with the right boundary (see Fig. 3). When $t_1 > t_0$, the unit-cell associated with the left boundary is in the topological phase and the one associated with the right boundary is in the trivial phase. This again makes perfect sense since it can be seen that the edge state appears on the left boundary. In contrast, when $t_1 < t_0$, the unit-cell associated with the left boundary is in the trivial phase while the one associated with the right boundary is in the topological phase, and thus the edge state would show up on the right boundary. Consequently, the bulk-edge correspondence indeed holds up well.

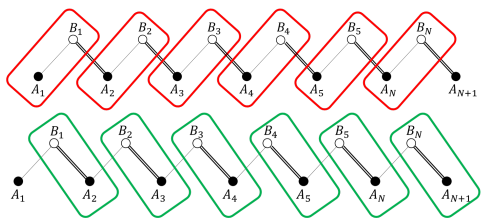



FIG. 3: Two possible ways to choose the unit cell, none of which can cover the whole system. Top: The unit cell that is consistent with the left edge of the system. Bottom: The unit cell that is consistent with the right edge.

The bulk-edge correspondence seen in the SSH model may be generalized to systems with next to nearest neighbor hopping amplitudes, which we call the extended SSH models. To be specific, let's consider the following two types of the extended SSH model. The Hamiltonians are given by

$$H_{\mathrm{ext1}} = \sum_{j=-\infty}^{\infty} \left\{ \left( t_0 A_j^\dagger + t_1 A_{j+1}^\dagger + t_2 A_{j+2}^\dagger \right) B_j + \mathrm{h.c.} \right\}, \tag{17}$$

and

$$H_{\mathrm{ext2}} = \sum_{j=-\infty}^{\infty} \left\{ \left( t_{-1} A_{j-1}^\dagger + t_0 A_j^\dagger + t_1 A_{j+1}^\dagger \right) B_j + \mathrm{h.c.} \right\}, \tag{18}$$

respectively. The corresponding Bloch Hamiltonians are then given by

$$h_{\mathrm{ext1}}(k) = \left( t_0 + t_1 \mathrm{e}^{ik} + t_2 \mathrm{e}^{2ik} \right), \tag{19}$$

and

$$h_{\mathrm{ext2}}(k) = \mathrm{e}^{-ik} \left( t_{-1} + t_0 \mathrm{e}^{ik} + t_1 \mathrm{e}^{2ik} \right). \tag{20}$$

Note that in the type 1 extended SSH model if we rename $B_j$ and $A_{j+1}$ as $\tilde{A}_j$ and $\tilde{B}_j$ so that they are grouped into a unit cell instead, then $H_{\mathrm{ext1}}$ would become

$$\begin{aligned} \tilde{H}_{\mathrm{ext1}} &= \sum_{j=-\infty}^{\infty} \left\{ \left( t_0 \tilde{B}_{j-1}^\dagger + t_1 \tilde{B}_j^\dagger + t_2 \tilde{B}_{j+1}^\dagger \right) \tilde{A}_j + \mathrm{h.c.} \right\}, \\ &= \sum_{j=-\infty}^{\infty} \left\{ \left( t_0 \tilde{A}_{j+1}^\dagger + t_1 \tilde{A}_j^\dagger + t_2 \tilde{A}_{j-1}^\dagger \right) \tilde{B}_j + \mathrm{h.c.} \right\}. \end{aligned} \tag{21}$$

It is thus equivalent to $H_{\mathrm{ext2}}$ if we properly rename the hopping amplitudes. Consequently, once we classify the type 1 extended SSH model, it is straight forward to see the corresponding classification of the type 2 extended SSH model.

Without lost of generality, we may rewrite

$$h_{\mathrm{ext1}}(k) = t_2 \left( \mathrm{e}^{ik} - \mathfrak{s}_1 \right) \left( \mathrm{e}^{ik} - \mathfrak{s}_2 \right), \tag{22}$$

with

$$\mathfrak{s}_1 = \frac{-t_1 + \sqrt{t_1^2 - 4t_0 t_2}}{2t_2}, \ \mathfrak{s}_2 = \frac{-t_1 - \sqrt{t_1^2 - 4t_0 t_2}}{2t_2}. \tag{23}$$

The equation in eq. (4) may be easily generalized to the current case, and we have

$$\nu = \frac{1}{2\pi} \int_0^{2\pi} dk \left\{ \frac{\mathrm{e}^{ik}}{\mathrm{e}^{ik} - \mathfrak{s}_1} + \frac{\mathrm{e}^{ik}}{\mathrm{e}^{ik} - \mathfrak{s}_2} \right\}. \tag{24}$$

Whenever $|\mathfrak{s}_i| < 1$, the point $\mathfrak{s}_i$ will be enclosed by the unit circle, and the corresponding integral will contribute 1 to the winding number $\nu$. On the other hand, it is known that the energy eigenstates of the right semi-infinite chain may be found by solving the following recurrence relation and boundary condition

$$\begin{aligned} &EA_j - (t_0 B_j + t_1 B_{j-1} + t_2 B_{j-2}) = 0; \\ &EB_j - (t_0 A_j + t_1 A_{j+1} + t_2 A_{j+2}) = 0, \\ &B_0 = B_{-1} = 0. \end{aligned} \tag{25}$$

In particular, it has been shown in Ref.[7] that the chiral zero modes are given by the solutions of the following characteristic equation

$$t_0 + t_1 s + t_2 s^2 = t_2 \left( s - \mathfrak{s}_1 \right) \left( s - \mathfrak{s}_2 \right) = 0, \tag{26}$$

which satisfy the condition

$$|\mathfrak{s}_i| < 1, \tag{27}$$

so that the corresponding wave function is normalizable.

From the above analysis, it is transparent to see there is a one-to-one correspondence between the winding number and the number of edge states, i.e. the bulk-edge correspondence. Factoring $h_{\mathrm{ext1}}(k)$ in a different way:

$$h_{\mathrm{ext1}}(k) = \mathrm{e}^{ik} \left( t_2 \mathrm{e}^{ik} + t_1 + t_0 \mathrm{e}^{-ik} \right), \tag{28}$$

we see that the factor $\mathrm{e}^{ik}$ would always contribute 1 to the winding number. Meanwhile, since

$$\begin{aligned} & t_2\mathrm{e}^{ik} + t_1 + t_0\mathrm{e}^{-ik} \\ &= t_1 + (t_2+t_0)\cos k + i(t_2-t_0)\sin k, \end{aligned} \tag{29}$$

the factor would have vanishing contribution to the winding number if

$$|t_2 + t_0| < t_1. \tag{30}$$

In contrast, if

$$|t_2 + t_0| > t_1, \tag{31}$$

the factor would contribute 1 and -1 to the winding numbed for $t_2 - t_0 > 0$ and $t_2 - t_0 < 0$, respectively. According to the winding number, the system can thus be classified into the following three categories:

i.) $|\mathfrak{s}_1| < 1, |\mathfrak{s}_2| < 1$, ($|t_2 + t_0| > t_1$, and $t_2 - t_0 > 0$): The system is in the topological phase with winding number $\nu = 2$. In this case, there should be two edge states on a boundary and they are described by

$$A_j = \alpha_1 s_1^j + \alpha_2 s_2^j,\ B_j = 0. \tag{32}$$

ii.) $|\mathfrak{s}_1| < 1, |\mathfrak{s}_2| > 1$, ($|t_2 + t_0| < t_1$): The system is in the topological phase with $\nu = 1$. In this case, there should be one edge state on a boundary and it is given by

$$A_j = \alpha_1 s_1^j,\ B_j = 0. \tag{33}$$

iii.) $|\mathfrak{s}_1| > 1, \mathfrak{s}_2| > 1$, ($|t_2 + t_0| > t_1$, and $t_2 - t_0 < 0$): The system is in the trivial phase with $\nu = 0$, and there would be no edge state on the boundary.

Again, the correspondence may be confirmed numerically by considering a finite chain of the extended SSH model. As an illustration, let's first consider the case that there are 60 (even) number of sites. In particular, we choose $(t_0, t_1, t_2) = (5, 10, 15)$ and $(t_0, t_1, t_2) = (5, 20, 10)$ so that the winding numbers are $\nu = 2$ and $\nu = 1$, respectively. The energy spectrum and the wave functions of the edge states for the two cases are shown in Fig.4 and Fig.5. Since the numbers of the left and right edge states are the same, all the edge states in these cases are mixing of the left and right ones similar to the SSH model.

Next, let's consider the case that there are 61 (odd) number of sites. Similar to the SSH model, the unit cells consistent with the left and right boundaries are different. From eq. (21), we now have

$$\tilde{h}_{\text{ext1}}(k) = \left(t_0\mathrm{e}^{ik} + t_1 + t_2\mathrm{e}^{-ik}\right) = \mathrm{e}^{ik}\bar{h}_{\text{ext1}}(k). \tag{34}$$

As a result, $\tilde{\nu} = 1 - \nu$. In other words, the winding numbers of the two edges are related by

$$\nu_{\text{left}} = 1 - \nu_{\text{right}}. \tag{35}$$

In the case $(t_0, t_1, t_2) = (5, 10, 15)$, we have $\nu_{\text{left}} = 2$ and $\nu_{\text{right}} = -1$. According to the bulk-edge correspondence, there should be two and one edge states on the left and right boundaries, respectively. The energy spectrum and the wave functions of the three edge states are shown in Fig.6. We expect one of the left edge states should have exact zero energy and is decoupled from that of the right boundary. This indeed can be seen in Fig.6

For $(t_0, t_1, t_2) = (10, 20, 5)$, we have $\nu_{\text{left}} = 1$ and $\nu_{\text{right}} = 0$. According to the bulk-edge correspondence, there should be only one edge states on the left boundary. The energy spectrum and the wave functions of the edge states are shown in Fig.7. Similarly, we expect the left edge states should have exact zero energy and is decoupled from the right boundary.

We may make further generalization by including next next to nearest neighbor hoping amplitudes and so on such that the corresponding Bloch Hamiltonian takes the form

$$\mathcal{H}(k) = \begin{pmatrix} 0 & \bar{h}(k) \\ h(k) & 0 \end{pmatrix}, \tag{36}$$

with

$$h(k) = \sum_{n=-n_-}^{n_+} t_n e^{ink}. \tag{37}$$

The range of the winding number $\nu$ would now become $[-n_-, n_+]$ [8].

## III. The Zak phase

In the literature, there is another physical quantity that is used to characterize the topological property of a 1-d systems, the Zak phase [4]:

$$\gamma_n = \frac{i}{2\pi}\int_0^{2\pi} dk \langle u_{k,n}\,|\partial_k|\,u_{k,n}\rangle. \tag{38}$$

Here,$|\ u_{k,n}\rangle$ are the Bloch states with $n$ the band index. The Zak phase has been shown to be related to the modern polarization [9]. According to conventional wisdom, the Zak phase is only summed over those bands that lie below the Fermi surface[6]. In particular, when one considers the SSH model, only the contribution of the lower band is taken into account. One of the reasons for such a practice comes from the fact that in the case of the 2-d Chern insulator if we sum over both bands, the total Berry flux is always zero. Obviously, such a quantity cannot give rise to any meaningful classification of topological insulators. However, we will show later on that the situation is quite different in 1-d systems.

It is known that there are some nuisances of the Zak phase. First of all, $\gamma_n$ is well-defined only up to integer multiple of $\pi$ due to the existence of gauge symmetry. Moreover, it is quantized only when there is

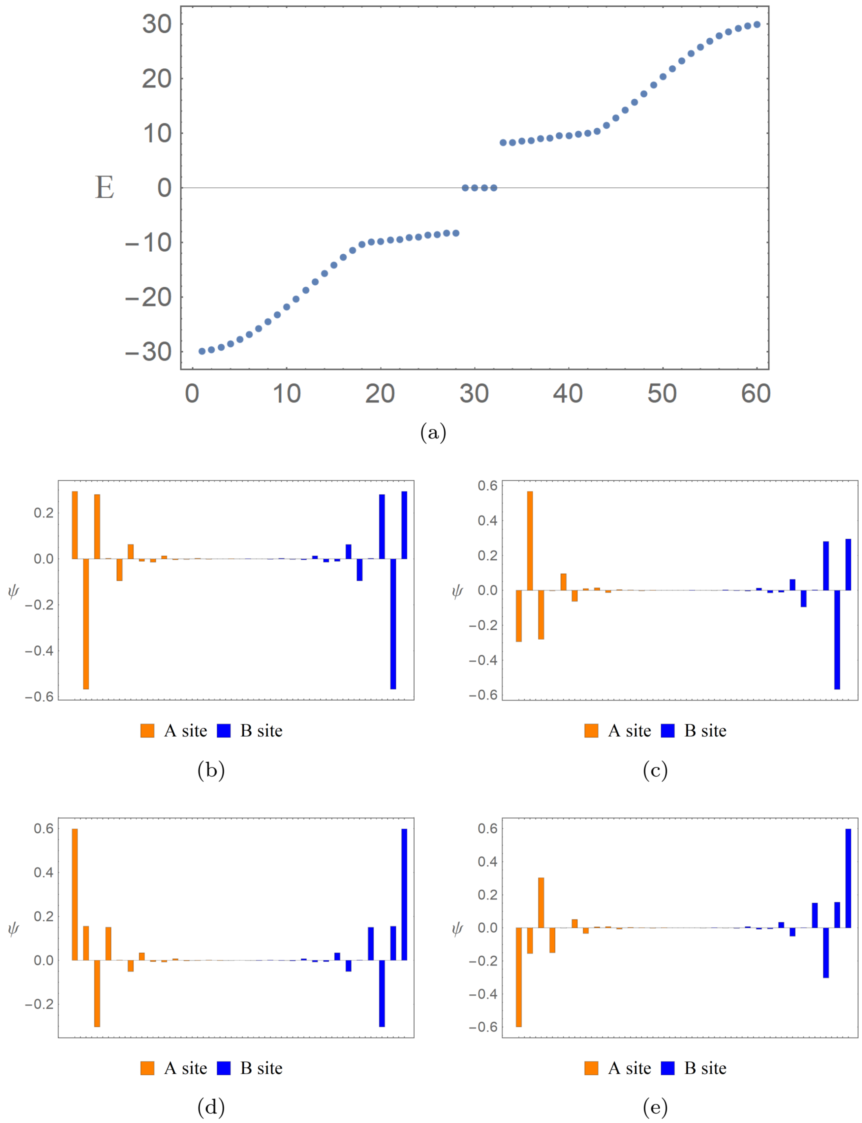



FIG. 4: (a)The energy spectrum of the extended SSH model with $\nu = 2$, where $(t_0, t_1, t_2)$ are $(5, 10, 15)$. (b)-(e) The wave functions of the four edge states with almost zero energy in the system.

chiral symmetry in the system[6]. If we think about the whole matter carefully, there is something unnatural about summing over only the bands below the Fermi surface. Whether a system is in the topological phase or not should be an intrinsic property of the whole system. Thus, all the bands should play a role in determining the phase that the system is in. Furthermore, if the Zak phase is relevant in any way to the topological property of a system, how can it be not quantized? In order to get rid of these rather awkward properties of the Zak phase, we propose to modify its definition to summing over all the bands. We will show that when we use this modified definition, the Zak phase will always be quantized independent of whether there is chiral symmetry in the system. To prove our points, let's consider a general two-band model with the following Bloch Hamiltonian

$$\mathcal{H} = \begin{pmatrix} m_0 & \bar{h}(k) \\ h(k) & -m_0 \end{pmatrix}. \tag{39}$$

Here, $h(k) = d_x(k) + id_y(k)$ and $m_0, -m_0$ are the on-site energy on the $A$ and $B$ sites, respectively. Consequently, chiral symmetry would be lost in general. The energy of the states in the upper and lower bands would be given by

$$E_{\pm} = \pm\omega(k), \tag{40}$$

with

$$\omega(k) = \sqrt{m_0^2 + |h(k)|^2}. \tag{41}$$

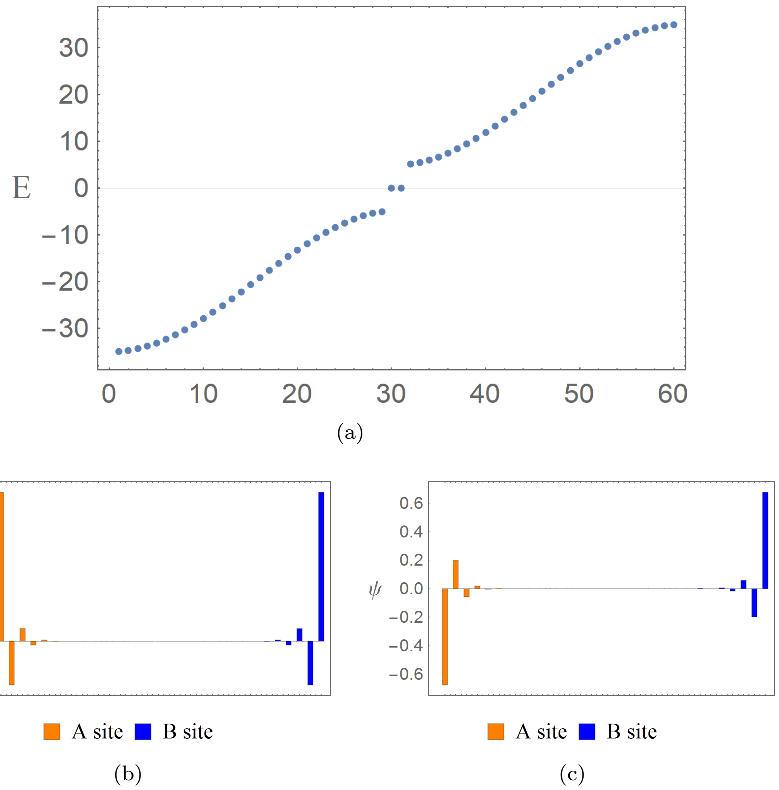



FIG. 5: (a)The energy eigenvalue of the system with $\nu = 1$, where $(t_0, t_1, t_2)$ are $(5, 20, 10)$. (b),(c) The wave functions of the two edge states with almost zero energy in the system.

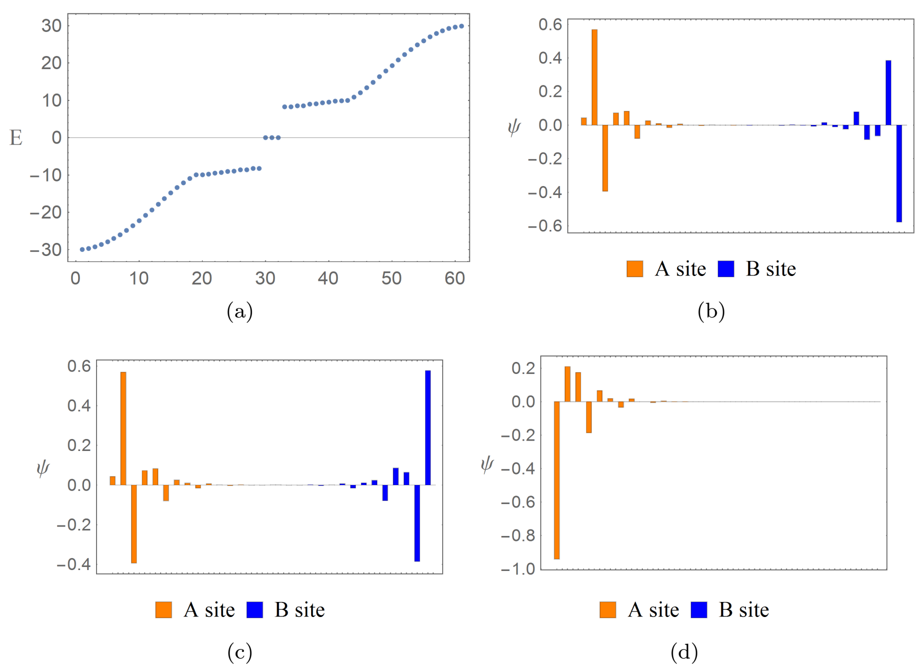


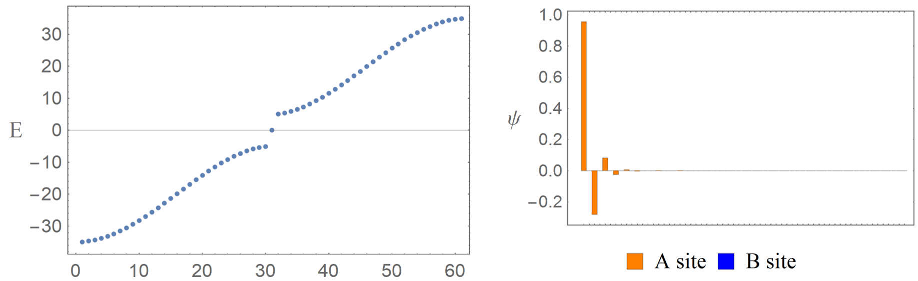

FIG. 6: (a)The energy spectrum of the system for the case that $(t_0, t_1, t_2) = (5, 10, 15)$ and the total number of sites is 61. (b),(c) The wave functions of the edge states with almost zero energy in the system. (d)The edge state with exact zero energy in the system.

The energy eigenstates may be chosen to be

$$|k, \pm\rangle = \frac{1}{\mathcal{N}_\pm} \begin{pmatrix} \bar{h} \\ \pm\omega - m_0 \end{pmatrix}, \tag{42}$$

where

$$\mathcal{N}_\pm = \sqrt{\omega(\omega \mp m_0)}. \tag{43}$$




(a) (b)

FIG. 7: (a)The energy spectrum of the system for the case that $(t_0, t_1, t_2) = (5, 20, 10)$ and the total number of sites is 61. (b) The edge state wave function with zero energy in the system.

Taking derivative on the energy eigenstates $|k, \pm\rangle$, we have

$$\partial_k |k, \pm\rangle = \frac{1}{\mathcal{N}_\pm^2} \begin{pmatrix} \bar{h}'\mathcal{N}_\pm - \bar{h}\mathcal{N}_\pm' \\ (\pm\omega - m_0)'\mathcal{N}_\pm - (\pm\omega - m_0)\mathcal{N}_\pm' \end{pmatrix}, \quad (44)$$

By making use of eq. (41) and (43), it can be seen after some algebra that

$$\begin{aligned} \gamma_\pm &\equiv i\int_0^{2\pi} dk\, \langle k, \pm |\partial_k|\, k, \pm\rangle \\ &= i\int_0^{2\pi} dk \frac{(h\bar{h}' - h'\bar{h})}{4\omega\,(\omega \mp m_0)}. \end{aligned} \quad (45)$$

If $m_0 = 0$ so that there is chiral symmetry in the symmetry, one see that since $\omega = |h|^2$

$$\gamma_+ = \gamma_- = -i\int_0^{2\pi} dk \left(\frac{h'}{4h} - \frac{\bar{h}'}{4\bar{h}}\right) = \nu\pi, \quad (46)$$

and thus are quantized. On the other hand, if $m_0 \neq 0$, it is obvious that they are generally different and not quantized. It is known that there is also an inversion symmetry (a crystalline symmetry) $\mathcal{I} = \tau_1$ in the SSH model in addition to the chiral symmetry. The Bloch Hamiltonian is invariant under the action of $\mathcal{I}$ : $\mathcal{I}\,\mathcal{H}(k)\,\mathcal{I}^{-1} = \mathcal{H}(-k)$. This was used in the literature to argued why the Zak phase is quantized in the case $m_0 = 0$ and that the SSH model is an example of topological crystalline insulators[3]. However, this is not very convincing since when the inversion symmetry is broken the chiral symmetry will be broken as well. Therefore, it is hard to see clearly which of the two symmetries is in action here.

If we sum over the two bands, we then obtain by using eq. (41) that

$$\gamma = \sum_{n=\pm} \gamma_n = -i\int_0^{2\pi} dk \left(\frac{h'}{2h} - \frac{\bar{h}'}{2\bar{h}}\right) = 2\pi\nu, \quad (47)$$

where $\nu$ is the winding number. Thus, it is now always multiple of $2\pi$. Even though the chiral symmetry and the inversion symmetry are generally both broken in the above Bloch Hamiltonian, the generalized Zak phase is still proportional to the winding number $\nu$. Moreover, we will show that there is still a bulk-edge correspondence for the modified Zak phase and the corresponding $\nu$ again indicates the number of edge states. This seem to be in contradiction with the periodic table of topological insulators and superconductors, since 1-d systems without chiral symmetry are classified as trivial [10]. One possible explanation for this is that maybe there is a crystalline symmetry in the system yet to be identified [11].

For simplicity, we will first use the Rice-Mele model so that $h(k) = t_0 + t_1 \mathrm{e}^{ik}$ to illustrate the above results. By introducing periodic time-dependence in the parameters $t_0, t_1$ and $m_0$, the model may be used to describe the charge-pumping process in the SSH model, which is in turn related to a 2-d Chern insulator [3]. However, as we shall show it can be seen as a 1-d topological insulator in its own right. Just like the SSH model, the system is in the topological phase when $t_1 > t_0$. When we consider a right semi-infinite chain of such a model, the recurrence relation and boundary condition are given by

$$\begin{aligned} &(E - m_0)\, A_j + (t_0 B_j + t_1 B_{j-1}) = 0; \\ &(E + m_0)\, B_j + (t_0 A_j + t_1 A_{j+1}) = 0, \\ &B_0 = 0. \end{aligned} \quad (48)$$

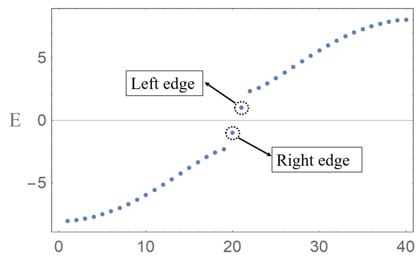
Thus, an edge state exists only if $t_1 > t_0$. Because of the existence of on-site energy, the energy of the edge state is now shifted to

$$E = m_0, \quad (49)$$

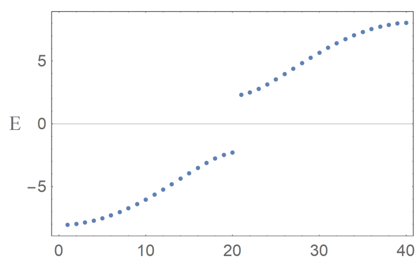
and the wave function of the edge state is given by

$$A_j = A_1\,(-t_0/t_1)^{j-1}\,,\; B_j = 0, \quad (50)$$

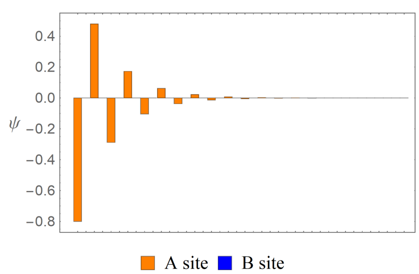
with $j \geq 1$. Similarly, an edge state exists only if $t_1 < t_0$ when a left semi-infinite chain is considered. Thus, the bulk-edge correspondence again holds up just like the SSH model, which may be verified numerically by considering a finite chain of such a system. Here, the number of sites is chosen to be 40 (even). The energy spectrum for the topological and trivial phases and the wave function of the edge states are shown in Fig.8. Note that the energies of the left and edge states are $m_0$, and $-m_0$, respectively. This in fact is consistent with the results obtained in Ref. [12]. Since the two edge states have different energies, they are not mixed in contrast to the SSH model.



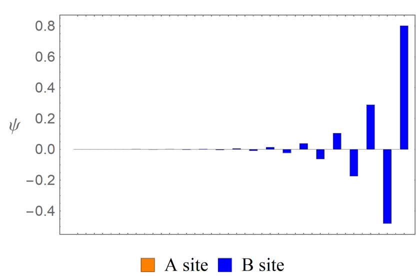

(a)




(b)




(c)




(d)

FIG. 8: (a)The energy spectrum in the topological phase of the Rice-Mele model, where $(t_0, t_1, m_0) = (3, 5, 1)$. The energies of the left and right edge states are $m_0$, and $-m_0$, respectively. (b) The energy spectrum in the trivial phase, where $(t_0, t_1, m_0) = (5, 3, 1)$. (c), (d) The wave functions of the two edge states in the system.

The above results, including the bulk-edge correspondence, may also be generalized to the extended Rice-Mele models in which there are next to nearest neighbor hopping amplitudes in the system, since the formula in (47) holds for a general $h(k)$. To be specific, let's again consider the case $h(k) = \left(t_0 + t_1 \mathrm{e}^{ik} + t_2 \mathrm{e}^{2ik}\right)$. Similar to the case of type 1 extended SSH model, the energy eigenstates of the right semi-infinite chain may be found by solving the following recurrence relation and boundary condition

$$\begin{aligned} &(E - m_0)A_j - (t_0 B_j + t_1 B_{j-1} + t_2 B_{j-2}) = 0; \\ &(E + m_0)B_j - (t_0 A_j + t_1 A_{j+1} + t_2 A_{j+2}) = 0, \\ &B_0 = B_{-1} = 0. \end{aligned} \tag{51}$$

Again, the system may be classified according to the modified Zak phase and there are also three categories:

i.) $|\mathfrak{s}_1| < 1, |\mathfrak{s}_2| < 1$, ($|t_2 + t_0| > t_1$, and $t_2 - t_0 > 0$): The system is in the topological phase with winding number $\nu = 2$. Again, there are on the boundary two edge states described by

$$A_j = \alpha_1 s_1^j + \alpha_2 s_2^j, \; B_j = 0. \tag{52}$$

ii.) $|\mathfrak{s}_1| < 1, |\mathfrak{s}_2| > 1$, ($|t_2 + t_0| < t_1$): The system is in the topological phase with $\nu = 1$. Here, there is on the boundary only one edge state given by

$$A_j = \alpha_1 s_1^j, \; B_j = 0. \tag{53}$$

iii.) $|\mathfrak{s}_1| > 1, \mathfrak{s}_2| > 1$, ($|t_2 + t_0| > t_1$, and $t_2 - t_0 < 0$): The system is in the trivial phase with $\nu = 0$, and there would be no edge state on the boundary.

Most of the results in the type 1 extended SSH model may be carried over except that the energy of edge states are now shifted to $E = m_0$ and $-m_0$, respectively. Numerical calculation have been done in finite chains to confirm the predictions. Again, one important difference from the previous results is that the edge states on the left and right boundaries have no mixing since their energies are different. First, let's consider the case that the number of sites is 40 (even). The energy spectrum for the topological phase with $\nu = 2$ and the wave functions of all the edge states are shown in Fig.9.

Next, let's consider the case that the number of sites is 41 (odd), and the hopping amplitudes $t_0, t_1, t_2$ remain the same so that $\nu_{\text{left}} = 2$ and $\nu_{\text{right}} = 1$. The corresponding energy spectrum and wave functions of the edge states are shown in Fig.10.

Because of the gauge ambiguity, the Zak phases of two sets of energy eigenstates related by a unitary transformation $|\mathbf{k}, \pm\rangle\!\rangle = \mathcal{U}\, |\mathbf{k}, \pm\rangle$ may differ by a multiple of $2\pi$:

$$\tilde{\gamma} = \gamma + \int_0^{2\pi} dk \, \mathrm{tr}\left(\mathcal{U}^\dagger \partial_k \mathcal{U}\right). \tag{54}$$

It is obvious that if $\mathcal{U} \in SU(2)$, then $\tilde{\gamma} = \gamma$. One example is the unitary transformation corresponding to the

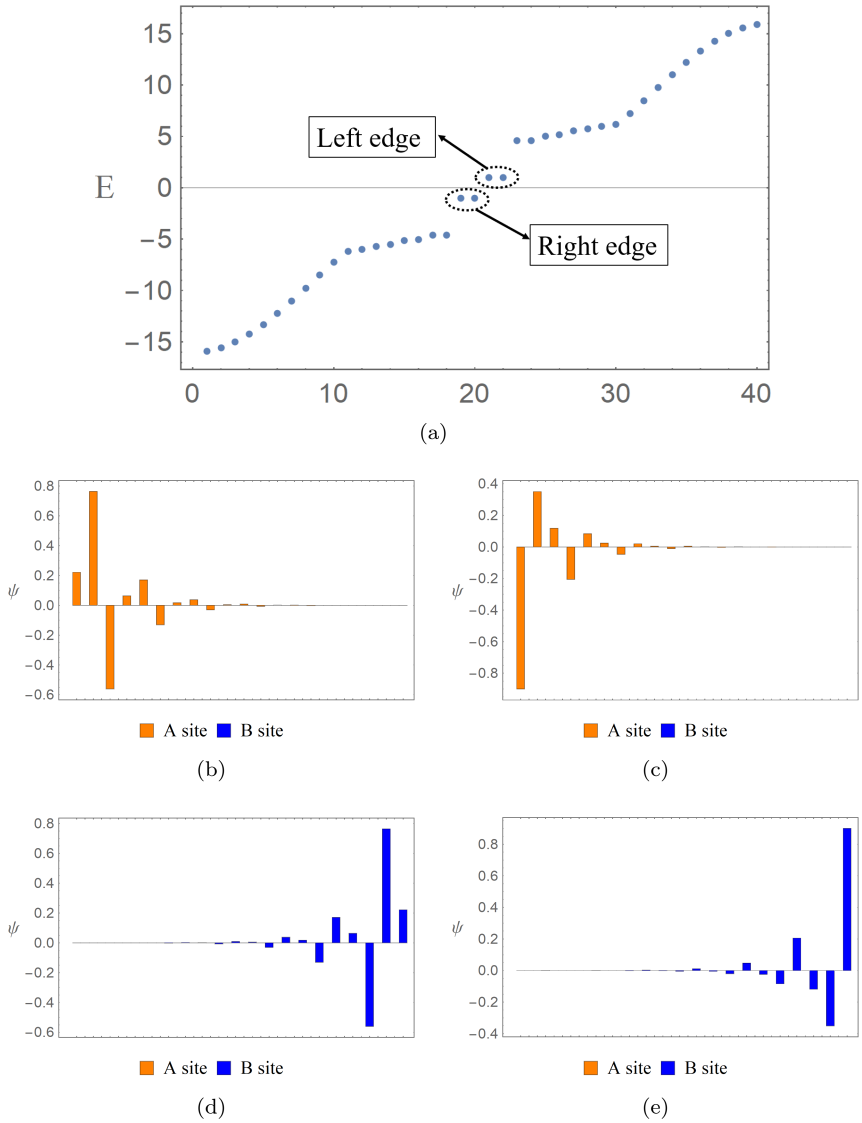



FIG. 9: (a)The energy spectrum in the topological phase of the extended Rice-Mele model with $(t_0, t_1, t_2, m_0) = (3, 5, 8, 1)$ and even number of sites so that $\nu_{\text{left}} = \nu_{\text{right}} = 2$. The energies of the left and right edge states are $m_0$ and $-m_0$, respectively. (b)-(e) The wave functions of the four edge states.

3-d rotation in the internal space, where $\mathcal{U} = e^{i(\theta/2)\hat{n}\cdot\vec{\tau}}$, with $\theta, \hat{n}$ specifying the magnitude and direction of the rotation. Therefore, non-trivial difference between $\tilde{\gamma}$ and $\gamma$ must be coming from the $U(1)$ part.

### IV. Conclusion and discussion

In this paper, we mainly focus on addressing two problems we encountered in 1-d topological insulators: 1. how to make sense of the bulk-edge correspondence in a finite chain of 1-d topological insulators, in which there are both the left and right boundaries. 2. how to modify the definition of the Zak phase so that it is always quantized and is explicitly related to some topological invariant, which allows a meaningful interpretation of the bulk-edge correspondence.

More specifically, we show in the first part that by choosing the unit cells so that they are consistent with the left and right boundaries of a finite chain, the bulk-edge correspondence would work perfectly. In particular, the winding numbers $\nu$ corresponding to the two unit cells may be used to count the numbers of edge states on the left and right boundaries, respectively. In the second part, we modify the definition of the Zak phase $\gamma$ to be summing over all the bands. We show for a general two-band model that the modified Zak phase satisfies $\gamma = 2\pi\nu$. Hence, it is always quantized independent of whether there is chiral symmetry in the system or not. According to the periodic table, 1-d system without chiral symmetry should be in the trivial class. However, we do

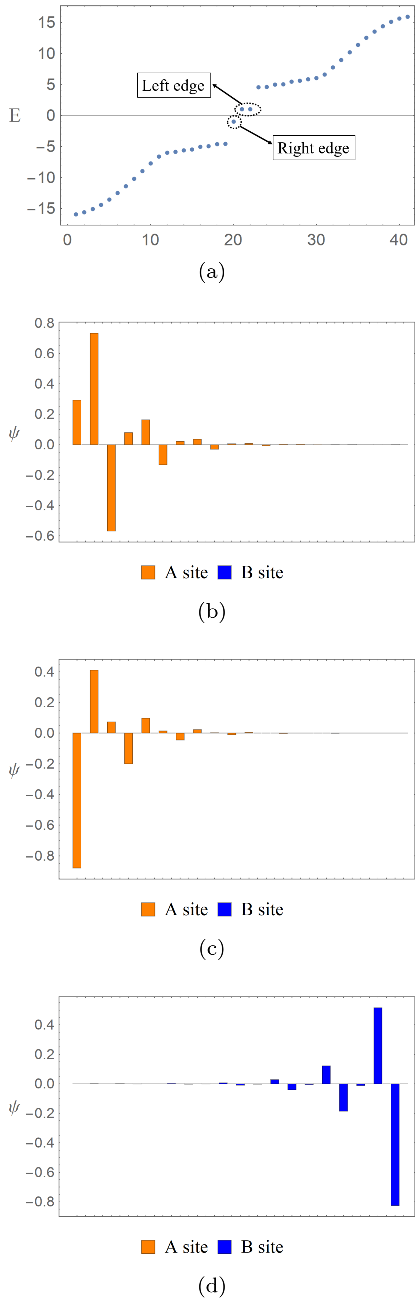



FIG. 10: (a)The energy spectrum in the topological phase of the extended Rice-Mele model with $(t_0, t_1, t_2, m_0) = (3, 5, 8, 1)$ and odd number of sites so that $\nu_{\rm left} = 2, \nu_{\rm right} = 1$. The energies of the left and right edge states are $m_0$ and $-m_0$, respectively. (b)-(d) The wave functions of the three edge states.

find some of these systems nonetheless have topological phases. Thus, we suspect there exists some yet to be identified crystalline symmetry in these systems.

It is well-known that the graphene Hamiltonian may be cast in the following form

$$H = \sum_{n_1,n_2} t\left\{A^\dagger_{n_1,n_2} + A^\dagger_{n_1+1,n_2} + A^\dagger_{n_1-1,n_2+1}\right\} B_{n_1,n_2} \\ +\text{h.c.}. \tag{55}$$

The location of an $A$ site is described by

$$\vec{r}_A = n_1\vec{a}_1' + n_2\vec{a}_2', \tag{56}$$

where we choose

$$\vec{a}_1' = a\Big(\frac{\sqrt{3}}{2}, \frac{1}{2}\Big),\ \vec{a}_2' = a\Big(\sqrt{3}, 0\Big), \tag{57}$$

for convenience. Note that $a = \sqrt{3}a_{\rm cc}$, with $a_{\rm cc} = 1.42\mathring{A}$, the carbon-carbon distance in graphene. In this convention, it would be straight forward to reduce the above Hamiltonian to those of the zigzag and armchair CNT's. See Fig. 11.

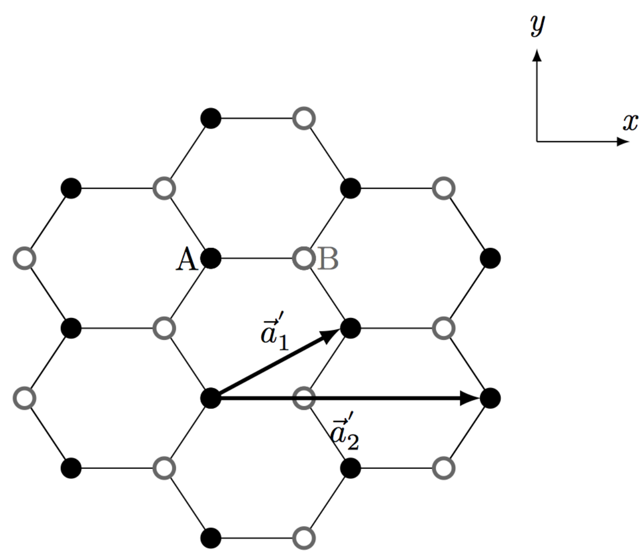



FIG. 11: Schematic diagram of graphene adopted from Ref. [13].

First, by imposing the periodic boundary condition along the $\vec{a}_1'$ direction in graphene, we obtain the Hamiltonian of the zigzag CNT:

$$H_{\rm zig} = \sum_{n_2} t\Big\{(1+e^{ik_1})A^\dagger_{n_2} + e^{-ik_1}A^\dagger_{n_2+1}\Big\}B_{n_2} \\ +\text{h.c.}. \tag{58}$$

Here, $k_1 = \frac{2\pi m_1}{aN_1}$ with $N_1$ the layer number along $\vec{a}_1'$ and $m_1 = 1, 2, ..., N_1$. It is obvious that the above Hamiltonian is closely related to that of the SSH model. It is transparent to see that the zigzag edge on the upper left boundary gives rise to the boundary conditions $B_0 = 0$. By adding an extra layer of B sites, the upper left boundary becomes the zigzag beard edge, which leads to the boundary conditions $A_0 = 0$. Meanwhile, the zigzag and zigzag beard edges on the lower right boundary give rise the boundary condition $A_{N_2+1} = 0$ and $B_{N_2+1} = 0$, respectively. It is quite obvious that the there are two transition points in $k_1$ that separate the topological and trivial phases. It is determined by the condition that

$$|1 + e^{ik_c}| = 1, \tag{59}$$

and thus $k_c = 2\pi/3, 4\pi/3$.

Next, by imposing the periodic boundary condition along the $\vec{a}_2'$ direction, we obtain the Hamiltonian of the armchair CNT:

$$H_{\mathrm{arm}} = \sum_{n_1} t\Big\{A_{n_1}^\dagger + A_{n_1+1,}^\dagger + e^{ik_2}A_{n_1-1}^\dagger\Big\}B_{n_1} + \mathrm{h.c.}. \tag{60}$$

Here, $k_2 = \frac{2\pi m_2}{\sqrt{3}aN_2}$ with $N_2$ the layer number along $\vec{a}_2'$ and $m_2 = 1, 2, ..., N_2$. Now, it can be seen that the above Hamiltonian resembles that of the type 2 extended SSH model. Again, it may be seen that on the lower boundary the armchair and armchair beard edges lead to the boundary condition $A_0 = 0, B_0 = 0$ and $B_0 = 0, B_{-1} = 0$, respectively. Of course, there is also a similar correspondence between the edges and boundary conditions on the upper boundary. According to what we have shown in Sec. II, the $h$ in the Bloch Hamiltonian associated with the armchair edge is given by

$$h(k_1) = t\left(1 + \mathrm{e}^{ik_1} + \mathrm{e}^{-ik_1-ik_2}\right), \tag{61}$$

where $k_2$ is a good quantum number and should be considered a constant. When $k_1$ goes over the Brillouin zone, $h(k_1)$ trace out a straight line. Since the corresponding winding number is zero, a CNT with the armchair edge is usually known to be in the trivial phase. On the other hand, the Bloch Hamiltonian associated with the armchair beard edge is given by

$$\tilde{h}(k_1) = t\left(\mathrm{e}^{ik_1} + \mathrm{e}^{2ik_1} + \mathrm{e}^{-ik_2}\right). \tag{62}$$

Define $\tilde{h}_a = \mathrm{e}^{ik_1} + \mathrm{e}^{2ik_1}$ and $\tilde{h}_b = -\mathrm{e}^{-ik_2}$. From Fig. 12, we see that except for the point $k_2 = 0$, the winding number is always 1 and there would be edge states on the corresponding boundary.

From the above analysis, we see that the results we obtained in Sec. II may be used to understand when and how the edge states in a CNT with various edges would appear. It is likely that similar understanding may be generalized to the counting of the number of edge states in the carbon nano-ribbons [14].

The Rice-Mele model have been used to relate the SSH model to the 2-d Chern insulator, which is characterized by the 2-d Chern number. On the other hand, we have shown in Sec. III that the Rice-Mele model may be classified by the Zak phase or the 1-d winding number. It would be interesting if we can find an explicit way to use the Zak phase to understand the 2-d Chern number or vice versa.

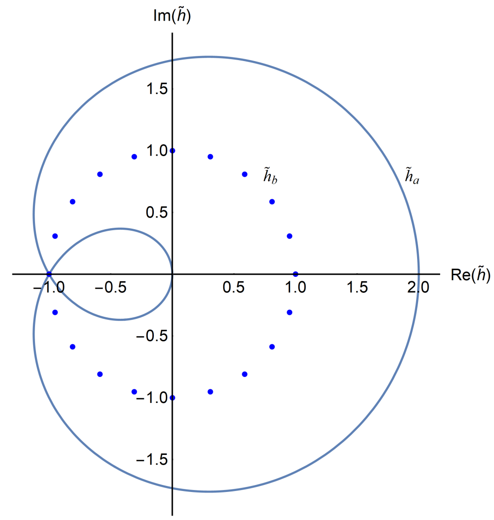



FIG. 12: Trajectory of $\tilde{h}_a$ and $\tilde{h}_b$. The winding number is always 1 on the armchair beard edge except for $k_2 = 0$.

## Acknowledgments

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[1] M. Z. Hasan and C. L. Kane, Rev. Mod. Phy., **82**, (2010); X.-L. Qi and S.-C. Zhang, Rev. Mod. Phy., **83**, (2011).
[2] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. **42**, 1698, (1979).
[3] J. K. Asboth, L. Oroszlany, and A. Palyi, arXiv:1509.02295.
[4] J. Zak, Phys. Rev. Lett., **62**, 2747, (1989).
[5] M. V. Berry, Proc. R. Soc. Lond. A. **392**, 45, (1984).
[6] J.-W. Rhim, J. Behrends, and J. H. Bardarson, Phys. Rev. B **95**, 035421 (2017).
[7] H. C. Kao, Phys. Rev. B **90**, 245435 (2014).
[8] B.-H. Chen, and D.-W. Chiou, arXiv: 1705.06913.
[9] R. D. King-Smith and D. Vanderbilt, Phys. Rev. B **47**, 1651 (1993); D. Vanderbilt and R. D. King-Smith, Phys. Rev. B **48**, 4442 (1993).
[10] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Phys. Rev. B 78, 195125 (2008); A. Kitaev, AIP Conf. Proc. 1134, 22 (2009); A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, AIP Conf. Proc. 1134, 10 (2009).
[11] L. Fu, Phys. Rev. Lett. **106**, 106802, (2011); T. Neupert and F. Schindler, arXiv: 1810.0348.
[12] R. S. K. Mong and V. Shivamoggi Phys. Rev. B **83**, 125109 (2011).
[13] L. E. F. Foa Torres, S. ROCHE, and J.-C. Charlier, *Introduction to Graphene-Based Nanomaterials From Electronic Structure to Quantum Transport* (Cambridge university press 2014).

[14] Y.-L Lee, F. Zhao, T. Cao, J. Ihm, and S. G. Louie Nano Lett. **18**, 7247 (2018);K.-S. Lin and M.-Y. Chou, Nano Lett. **18**, 7254 (2018).