Topological phase transition between normal insulator and topological metal state in a quasi-one-dimensional system

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ABSTRACT

We theoretically report the finding of a new kind of topological phase transition between a normal insulator and topological metal state where the closing-reopening of bandgap is accompanied by passing the Fermi level through an additional band. The resulting nontrivial topological metal phase is characterized by stable zero-energy localized edge states that exist within the full gapless bulk states. Such states living on a quasi-one-dimensional system with three sublattices per unit cell are protected by hidden inversion symmetry. While other required symmetries such as chiral, particle-hole, or full inversion symmetry are absent in the system.

In recent years, the exploring of topological phases has been at the center of attention, in particular, in condensed matter systems.¹ The key feature is the emergence of symmetry protected gapless boundary modes due to topological bulk states. Topological phases mainly have been categorized into topological insulators²–⁵ and topological superconductors⁶ that are studied theoretically and experimentally. In contrast to these topological phases where edge states reside within the gap of bulk states, there are other types of unconventional topological phases known as topological semi-metals⁷ and topological metals (TMs).⁸,⁹ In the former, there exist band touching nodes at Fermi energy occurring in three dimensional noncentrosymmetric or magnetic materials. While the latter case, which can also take place in low-dimensional systems, has a finite Fermi surface.

Depending on the properties of edge states, topological semimetals and metals can be regarded as two types. First, while topological edge states remain isolated in the bandgap, Fermi level crosses bulk and edge states at different momenta (quantum numbers). This situation, for instance, has been reported in TMs,⁸ semimetals,¹⁰ and even in a narrow energy window of topological insulators.¹¹ Second, gapless edge states coexist with gapless bulk states such that some edge and bulk states would have not only the same energy but also the same momentum (quantum number). This phase has been investigated in a quasi-one-dimensional (1D) system¹⁸ where the finite-energy edge states can penetrate into bulk states hybridizing with them¹² and in a 1D system where the coexistence of edge and bulk states occurs at Fermi energy in a single point of parameter space.⁹ However, this kind of TM phase deserves to be investigated further with a more stable feature.

Often, on the other hand, topological superconducting or insulating phase can be settled down, respectively, on the trivial superconductor or insulator through occurring topological phase transition when band inversion takes place. Furthermore, in previous works, it has been shown that the TM phase can be established on the trivial metallic ground state through closing-reopening of subband gap⁸ or main bandgap.⁵ So, it is indeed intriguing to have a situation in which the underlying state of matter in nontrivial and trivial topological phase of a system belonging to different states can be related to each other, possibly, with a new kind of topological phase transition.

In this paper, within the tight-binding approach in a quasi-1D model with three sublattices per unit cell (Fig. 1), the occurrence of a new kind of topological phase transition between normal insulator (NI) and TM is investigated. Interestingly, in such phase transition in addition to gap closing-reopening between two bands, another band passes the Fermi level (Fig. 2) resulting in the emergence of zero-energy edge states within bulk states (Fig. 3(a)). Although the system has no explicit symmetry, in a subspace of the Hilbert space, there is a hidden inversion symmetry protecting the TM phase.
The model we consider is a three-component quasi-1D lattice as represented in Fig. 1. Using the tight-binding theory, the Hamiltonian of system can be defined as

$$H = \sum_{n=1}^{N} t_1 (A_n^\dagger B_n + B_n^\dagger C_n + A_n C_n) + \sum_{n=1}^{N-1} t_2 (A_n^\dagger A_{n+1} + B_n^\dagger B_{n+1}) + \frac{1}{2} \sum_{n=1}^{N-1} t_2 (C_n^\dagger A_{n+1} + C_n B_{n+1}) + \text{h.c.}$$

(1)

where $X_n^\dagger$ ($X_n$) is the creation (annihilation) operator on the sublattice $X = A, B, C$ of the $n$th unit cell and $N$ is the number of unit cell. Also, $t_1 = t(1 + \delta_1)$ is intra unit cell hopping and $t_2^{(\pm)} = t(1 - (+)\delta_2^{(\pm)})$ is oblique (horizontal) inter unit cell hopping to the nearest neighbors. $\delta_1$ and $\delta_2^{(\pm)}$ are some parameters modulating hopping energies. We choose $t$ as the unit of energy.

With periodic boundary conditions, $H$ is invariant under translations by a unit cell. So, after Fourier transformation, the Hamiltonian can be written in the basis of $\psi_k = (A_k, B_k, C_k)^\dagger$ yielding compact from $H = \sum_k \psi_k^\dagger \mathcal{H}(k) \psi_k$ with

$$\mathcal{H}(k) = \begin{pmatrix} 2t_1 \cos(k) & t_1 & t_1 + t_2 e^{i k} \\ t_1 & 2t_2 \cos(k) & t_1 + t_2 e^{-i k} \\ t_1 + t_2 e^{-i k} & t_1 + t_2 e^{i k} & 0 \end{pmatrix}$$

(2)

Diagonalizing Eq. (2) gets the eigenvalues,

$$E^0 = -2t_1 + \eta,$$

$$E^\pm = \frac{1}{2} \left( \eta \pm \sqrt{\eta^2 + 2(t_1^2 + 4t_2^2 + 8t_1t_2 \cos(k))} \right),$$

(3)

where $\eta = t_1 + 2t_2 \cos(k)$. The possibility of emerging topological phases though gap closing/reopening conditions at the $k_x = (0, \pi)$ would be provided if $E^+ = E^-$ leading to

$$t_1 = e^{i \theta} \frac{2}{9} (t_2^2 + 4t_2 \pm \sqrt{(-2t_1 + t_2)^2}).$$

(4)

Note, Eq. (4) implicates that topological phase transition is possible if the term under the square root is zero, i.e., $t_2^2 = t_2/2$. Under such condition, Eq. (4) indicates phase boundaries distinguishing topologically nontrivial phase from topologically trivial one.

In Fig. 2, we depicted the band structure of system showing closing and reopening of the energy gap between the two bands $E^+$ and $E^-$ near the topological phase transition point. In Fig. 2(a), the gap of system is open and there are no energy states at Fermi energy. So, the system is a NI. With increasing $t_1$, from Fig. 2(b), one can see that the gap closes leading to the topological phase transition. At the same time, surprisingly, the band $E^0$ shifts towards the Fermi level and touches it. After topological phase transition, as shown in Fig. 2(c), the energy gap between $E^+$ and $E^-$ is reopened and the band $E^0$ crosses the Fermi level which represents a metallic state. This signals that the whole system will be a conductor in a nontrivial topological phase giving rise a new type of topological phase transition from NI to TM phase.

As already mentioned above, if $t_2^2 \neq t_2/2$ the system does not support any topological phase. Because, in general, Hamiltonian (2) does not have chiral, particle-hole, and/or inversion symmetries. As such, the system provides a trivial phase
without any topological edge state in the gap or bulk states under the open boundary conditions. However, if \( t_2' = t_2/2 \) then inversion symmetry in a subspace of the Hilbert space of system would be revived (as will be discussed below) and Eq. (4) reduces to \( t_1 = t_2 e^{i k} \) reminiscing the gap closure condition of SSH model.\(^{13}\) So, hereafter, we set \( t_2' = t_2/2 \) otherwise specified.

Furthermore, Hamiltonian \( \mathcal{H}(k) \) has exchange symmetry with the corresponding exchange operator \( \Upsilon \) defined as,

\[
\Upsilon \psi_k = \psi_k^\prime = \begin{pmatrix} B_k \\ A_k \\ C_k \end{pmatrix},
\]

which exchanges the sublattices \( A \) and \( B \). Owing to the presence of such symmetry, \( [\mathcal{H}(k), \Upsilon] = 0 \), and then the Hamiltonian can be block-diagonalized in the basis of \( \Upsilon \) under the transformation \( \Upsilon^{-1} \mathcal{H}(k) \Upsilon = \mathcal{H}_{BD}(k) \) yielding

\[
\mathcal{H}_{BD}(k) = \begin{pmatrix} h_1 & 0 \\ 0 & h_2 \end{pmatrix},
\]

where

\[
h_1 = -2t_1 + \eta, \quad h_2 = \begin{pmatrix} \eta \\ \sqrt{2}(t_1 + t_2 e^{i k}) \end{pmatrix},
\]

and

\[
\Upsilon = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}.
\]

Note that the obtained bases of exchange operator (9) can be related to a unitary matrix in block-diagonalizing a class of quasi-1D and -2D systems comprised of odd chains.\(^{17,18}\) In fact, the block-diagonalization (6) splits the Hilbert space of the system into two subspaces so that one can examine their topological properties independently. Interestingly, in one of the subspaces, the subsystem \( h_2 \) can be regarded as generalized SSH model with next-nearest hopping, \( t_2' \), and on-site potential, \( t_1 \).\(^{19}\) Then, the subspace associated with \( h_2 \) would host topological phases which in combination with the metallic subspace of \( h_1 \) would make the whole system TM.

To discuss about the symmetry of the subsystem \( h_2 \) we rewrite its Hamiltonian as

\[
h_2 = h_0 \sigma_0 + \sum_i h_i \sigma_i,
\]

where \( \sigma_0 \) is identity matrix, \( \sigma_i \) is \( i (= x, y, z) \) component of Pauli matrices, and

\[
h_0 = h_z = \eta/2, \quad h_x = \sqrt{2} \eta, \quad h_y = \sqrt{2} t_2 \sin(k).
\]
It is well-studied that the simultaneous presence of all three components $h_x$, $h_y$, and $h_z$ in 1D two-band Hamiltonians, for instance, SSH model, breaks inversion symmetry and, subsequently destroys topological edge states.\textsuperscript{20} But, for our model although $h_z$ is nonzero, due to the relation $h_z = \frac{1}{2\sqrt{2}} h_x$, one can find effective inversion symmetry, $\Pi h_2(k)\Pi = h_2(-k)$, in the subspace of $h_2$ with inversion operator

$$\Pi = \frac{1}{3} \left( \begin{array}{cc} 1 & 2\sqrt{2} \\ 2\sqrt{2} & -1 \end{array} \right).$$  \hfill (14)

This implies that there exists a hidden inversion symmetry in the system protecting the topological phase. The emergence of inversion-symmetry-protected topological phase can be verified by quantized $\mathbb{Z}$ invariant.\textsuperscript{41}

Moreover, the $h_2$ has time-reversal symmetry fulfilling $\mathcal{T} h_2(k) \mathcal{T}^{-1} = h_2(-k)$ where the time-reversal operator is $\mathcal{T} = \sigma_0 \mathcal{X}$ with $\mathcal{X}$ being complex conjugate operator. Also, the reason for the breaking of chiral symmetry can also be seen from the energy dispersions of the two-band subsystem $h_2$ which are

$$E^\pm = h_0 \pm \sqrt{h_x^2 + h_y^2 + h_z^2} = \frac{h_x}{3} \pm \sqrt{\frac{9h_y^2}{8} + h_z^2}.$$  \hfill (15)

Here, the term $h_0$ breaks chiral symmetry so, as usual, one may expect that the zero-energy edge states will be shifted by this term. Nevertheless, interestingly, the relation between $h_0$ and $h_x$ holds the energy of edge states at zero energy which is in contrast to the previous studies. Therefore, due to $\mathcal{T}^2 = 1$ and $\Pi^2 = 1$, according to the modified periodic table,\textsuperscript{4,22,23} the symmetry class of subsystem $h_2$ is AI with topological index $\mathbb{Z}$.

The existence of the hidden inversion symmetry guarantees that the eigenvectors of $h_2$ have a well-defined parity at the inversion symmetric momenta $k_y = (0, \pi)$. So, one can define an integer invariant as $\mathbb{Z} = |n_0 - n_\pi|$ where $n_0$ and $n_\pi$ denote the number of negative parities at $k_y = 0$ and $k_y = \pi$, respectively.\textsuperscript{21} The analytical expression of topological invariant $\mathbb{Z}$ for the subsystem $h_2$ can be obtained as (for details see\textsuperscript{16})

$$\mathbb{Z} = \begin{cases} 0, & \text{if } \text{sgn}(\eta(0)) = \text{sgn}(\eta(\pi)) \\ 1, & \text{if } \text{sgn}(\eta(0)) \neq \text{sgn}(\eta(\pi)) \end{cases},$$  \hfill (16)

where $\text{sgn}(x)$ is the Sign function. For $\mathbb{Z} = 1$ a nontrivial topological phase will be revealed in the subspace of $h_2$. In such a situation, due to bulk-edge correspondence, the gapless edge states associated with the nontrivial topological character of bulk states will be appeared at the boundary of the system under open boundary conditions. For $\mathbb{Z} = 0$ the subsystem $h_2$ has a trivial phase.

Generally, combining the two-band subsystem $h_2$ with the single-band subsystem $h_1$ leads to another topological aspect for which gapped topological bands would coexist with trivial metallic band resulting in TM phase.\textsuperscript{8,9,12,17,18} This means that when the system has open boundary conditions, in the topologically nontrivial phase of $h_2$, there exist zero-energy edge states near the system boundaries while the subsystem $h_1$ has topologically trivial phase. So, the band structure of the whole system shows an interesting phenomenon that topological edge states of $h_2$ are in the metallic bulk states of $h_1$ instead of being in the system gap as will be shown below.

**Numerical results.**

To complement analytical results with numerical ones, we diagonalize the Hamiltonian (1) numerically under open boundary conditions. In order to identify the localized edge states penetrated into extended bulk states under open boundary conditions, in the following, we evaluate the inverse participation ratio (IPR) of states.\textsuperscript{24} The IPR for an eigenstate $\psi_E(j)$ in the corresponding eigen energy $E$ is given as

$$I_E = \frac{\text{Ln} \sum_j |\psi_E(j)|^4}{\text{Ln} 3N}.$$  \hfill (17)

If $\psi_E(j)$ is localized, then $I_E = 0$, whereas if $\psi_E(j)$ is extended, then $I_E = -1$.

The band structure of system along with its corresponding topological invariant $\mathbb{Z}$ as a function of $t_1$ is plotted in Figs. 3(a) and 3(b) for the cases $t_1^2 = t_2/2$ and $t_1^2 \neq t_2/2$, respectively. In Fig. 3(a), with establishing the hidden inversion symmetry due to $t_1^2 = t_2/2$, the gap of $h_2$ closes and then reopens at the topological phase transition points. Subsequently, the topological invariant takes 0 and 1 values for trivial and nontrivial regimes, respectively. In the nontrivial region, the system hosts the degenerate zero-energy edge states within the bulk states in a width range of $t_1$ indicating stable TM phase. Since, in the trivial region, the system is trivial insulator, as a result, a topological phase transition has occurred between NI and stable TM phase. Also, when $t_1^2 \neq t_2/2$, owing to violating the hidden inversion symmetry, as shown in Fig. 3(b), the degeneracy of edge states is
Figure 3. (Color online) Energy spectra with their relevant topological invariant as a function of $t_1$ under open boundary conditions for (a) $t'_2 = t_2/2$ and (b) $t'_2 \neq t_2/2 = -0.3$. Here, $t'_1 = -0.6t$. (c) Topological phase diagram as functions of intra and inter unit cell hoppings $t_1$ and $t_2$. The red region represents the nontrivial TM phase while the gray region indicates NI.

Figure 4. (Color online) Dependence of local density of states on $E$ and on unit cell index $x$ in (a) TM phase with $t_1 = -0.9t$ and (b) NI phase with $t_1 = -1.55t$. Here, $t'_2 = t_2/2 = -0.6t$.

Summary and discussion

We introduced a quasi-1D model that presents a new topological phase transition between the TM phase and NI. In such topological phase transition, in addition to bandgap closing-reopening, another band crosses the Fermi level. The Hamiltonian of system can be block-diagonalized into two subsystems in the presence of exchange symmetry. One of these subsystems can be regarded as the generalized SSH model hosting topological edge states when the band of other subsystem passes the Fermi level resulting in the TM phase. Finally, the edge states created in the absence of chiral or particle-hole symmetry and protected by the hidden inversion symmetry. By breaking the hidden inversion symmetry, depending on the parameter, the system has either NI or metallic state with nondegenerate trivial edge states.

Experimentally, our model can be realized by coupled acoustic resonators, topolectrical circuits, optical lattices, photonic crystals, and mechanical systems. Using cold atoms, it is possible to simulate quasi-1D chains and to reveal the topological features employing density and momentum-distribution measurements. Also, using spatially resolved
radio-frequency spectroscopy, the topological edge states can be probed by the LDOS.

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Author contributions
M. V. Hosseini conceived the idea of the research and directed the project. All authors developed the research conceptions, analysed, discussed the obtained results, and wrote the paper. M. Jangjan performed the calculations.

Additional information
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