Topological hierarchy insulators and topological fractal insulators

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Abstract – Topological insulators are new states of quantum matter with metallic edge/surface states. In this paper, we point out that there exists a new type of particle-hole symmetry-protected topological insulator — the topological hierarchy insulator (THI), a composite topological state of a (parent) topological insulator and its defect-induced topological mid-gap states. A particular type of THI is the topological fractal insulator, which is a THI with self-similar topological structure. In the end, we also discuss the possible experimental realizations of THIs.

Recently, new research has focused on searching for topologically nontrivial phases protected by symmetries. Topological band insulators (TBIs) provide an example of symmetry-protected topological states, in which there exist metallic edge/surface states [1,2]. According to the “ten-fold way” characterization of different symmetries [3], there are two types of TBIs in two dimensions (2D): a $Z$-type TBI with integer quantum Hall effect [4] and a $Z_2$-type TBI with quantum spin-Hall effect [1,5–8]. Researchers found that by extending the topological classification of band structures to include crystal point group symmetries, there exists a new type of TBI — topological crystalline insulators [9]. These additional symmetries lead to a nontrivial topology of bulk wave functions and gapless edge/surface states.

Because of the “holographic feature”, the nontrivial topological properties of TBIs can be detected by probing topological defects. For example, in two-dimensional $Z$-type TBIs, a $\pi$-flux traps mid-gap (MG) zero energy states (zero modes) [10–12]. For this topological state with a superlattice of $\pi$-fluxes, due to the polygon rule (each fermion gains an accumulated phase shift $|\phi| = (n - 2)\pi/2$ when encircling a smallest n-polygon [13]), the defect-induced mid-gap states can be regarded as an emergent “TBI” with nontrivial topological properties, including the nonzero Chern number and the gapless edge states [14].

In this paper we point out that a new type of topological insulator — topological hierarchy insulator — may exist in which the topological properties are protected by translational and (generalized) particle-hole symmetry. In this system, the nontopological defect — vacancy — traps zero mode [15]. For a system with a vacancy-superlattice (VSL), the ground state becomes a topological hierarchy insulator (THI). To show the nontrivial topological properties of THI, we take the Haldane model on a square lattice. –

The Haldane model on a square lattice. – Our starting point is the (spinless) Haldane model on a square lattice [16,17], the Hamiltonian is

$$
H_{\text{parent}} = -t \sum_{i \in A} \left( \hat{c}_{i+\hat{x}}^\dagger \hat{c}_i + i \hat{c}_{i+\hat{y}}^\dagger \hat{c}_i + \text{h.c.} \right) + t \sum_{i \in B} \left( \hat{c}_{i+\hat{x}}^\dagger \hat{c}_i - i \hat{c}_{i+\hat{y}}^\dagger \hat{c}_i + \text{h.c.} \right) - t' \sum_{i \in A} \left( \hat{c}_{i+\hat{x}+\hat{y}}^\dagger \hat{c}_i + \hat{c}_{i+\hat{x}+\hat{y}}^\dagger \hat{c}_i + \text{h.c.} \right) + t' \sum_{i \in B} \left( \hat{c}_{i+\hat{x}+\hat{y}}^\dagger \hat{c}_i + \hat{c}_{i+\hat{x}+\hat{y}}^\dagger \hat{c}_i + \text{h.c.} \right),
$$

(1)

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The site parameter is as a function of vacancy. (d) The energy splitting $\Delta E$ between two vacancies as a function of $L$ (the distance of two nearby vacancies). The parameter is $t' = 0.2t$.

where $\hat{c}_i$ is the annihilation operator of the fermions at the site $i$. $A$ and $B$ label the sublattices. $t$ and $t'$ are the nearest-neighbor (NN) and the next-nearest-neighbor (NNN) hopping parameters, respectively. For the Hamiltonian in eq. (1), there exists a $\pi$-flux in each square plaquette and a $\pi'$-flux in each triangular lattice. The illustration of the Haldane model on a square lattice is shown in fig. 1(a). In this paper, we set the lattice spacing $a$ to be unit.

For free fermions of the Haldane model on a square lattice, the energy spectrum is

$$E_k = \pm \sqrt{\xi_k + \xi_k'^2}$$

where $\xi_k = 4t^2[\sin^2(kx) + \sin^2(ky)]$ and $\xi_k' = 4t' \cos(kx) \cos(ky)$.

In particular, we point out that the Hamiltonian in eq. (1) has the particle-hole (PH) symmetry. Under PH transformation, we have

$$\hat{H}_{\text{parent}} = -\mathcal{P} \hat{H}_{\text{parent}} \mathcal{P},$$

where $\mathcal{P} = R \cdot K$ is the PH transformation operator [15,18].

Here, $R$ is an operator that leads to $\hat{c}_i \leftrightarrow (-1)^i \hat{c}_i^\dagger$ and $K$ is the complex conjugate operator. As a result, each energy level with positive energy $E$ is paired with an energy level with negative energy $-E$. Because the Hamiltonian in eq. (1) is on a bipartite lattice, the quantum levels of the system with a single vacancy become an odd number. As a result, there must exist an unpaired electronic state when we remove a lattice site to create a vacancy. Because of the PH symmetry, the corresponding unpaired electronic state must have exactly zero energy [15].

We have calculated the fermionic zero mode around a single vacancy by the exact diagonalization numerical approach on a $60 \times 60$ square lattices and give the particle density distribution around the vacancy in fig. 1(c). The particle density is localized around the vacancy center within a length scale $\xi \sim (\Delta f)^{-1}$ where $\Delta f$ is the fermion energy gap. We denote the wave function of the zero mode by $\psi_0(r_i - R)$ where $R$ is the position of the vacancy. The quantum states of the fermionic zero mode around a vacancy can be formally described in terms of the fermon Fock states $\{|0\}, |1\}$. Here, $|0\rangle, |1\rangle$ denote the empty state and the occupied state, respectively.

**Topological hierarchy insulator.** We next study the Haldane model with vacancy-superlattice. When there are two vacancies nearby, the inter-vacancy quantum tunneling effect occurs and the fermionic zero modes on two vacancies couple. The lattice constant of the VSL is denoted by $L$, which is the distance between two nearby vacancies. When the vacancies are located on different sublattices, the energy splitting $\Delta E$ is finite ($L/a$ is an odd number); when the vacancies are located on the same sublattice, the energy splitting vanishes, $\Delta E = 0$ ($L/a$ is an even number). The energy splitting $\Delta E$ between two vacancies as a function of $L$ is shown in fig. 1(d). When two vacancies are well separated (or $L \rightarrow \infty$), the quantum tunneling effect can be ignored and we have two quantum states with exact zero energy. In contrast, for the smaller $L$ (odd number times of $a$), the coupling between two zero modes becomes stronger and the energy splitting cannot be neglected.

For the case of $\xi < L$, we can consider each vacancy as an isolated “atom” with localized electronic states and use the effective tight-binding model to describe these quantum states induced by the VSL. We now construct the superpositions of the localized states to obtain the sets of Wannier wave functions $\psi_0(r_i - R)$. In general, the effective tight-binding model of the localized states induced by the VSL becomes

$$\hat{H}_{\text{1-VL}} = -\sum_{\langle R,R' \rangle} T_{RR'} \hat{d}_R^\dagger \hat{d}_{R'} - \sum_{\langle\langle R,R' \rangle\rangle} T'_{RR'} \hat{d}_R^\dagger \hat{d}_{R'}$$

$$- \sum_{\langle\langle\langle R,R' \rangle\rangle\rangle} T''_{RR'} \hat{d}_R^\dagger \hat{d}_{R'} + \ldots,$$

where $\hat{d}_R$ is the fermionic annihilation operator of a localized state on vacancy $R$. $T_{RR'}$, $(T'_{RR'}, T''_{RR'})$ is the hopping parameter between NN (NNN, NNNN) sites $R$ and $R'$ and is determined by the energy splitting $\Delta E$, $|T_{RR'}| = |\Delta E| / |\Delta E'|$, $|T'_{RR'}| = |\Delta E''|$. In general, because $|T''_{RR'}| \ll |T'_{RR'}|$, $|T_{RR'}|$ (see the energy

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The parameter is the square-VSL. (d) The edge states of mid-gap states. The \( \pi_L \) is just a particle’s hopping amplitude \(|\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + i\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + \text{h.c.}|\).

Because the energy splitting \( \Delta E \) only determines the particle’s hopping amplitude \(|\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + i\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + \text{h.c.}|\), we need to settle down the phase of \( T_{RR} \). In particular, to preserve PH symmetry, the total phase around a plaquette is \( \pi \) or 0. An approach is to count the total flux number inside the plaquette. For the mid-gap states induced by VSL, every four NN vacancies can be either \( \pi \) or 0. An approach is to count the total flux number inside the plaquette.

Because the energy splitting \( \Delta E \) only determines the particle’s hopping amplitude \(|\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + i\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + \text{h.c.}|\), we need to settle down the phase of \( T_{RR} \). In particular, to preserve PH symmetry, the total phase around a plaquette is \( \pi \) or 0. An approach is to count the total flux number inside the plaquette.

Based on the Haldane model, we studied the properties of a PH symmetry-protected TBI with VSL and introduce the concept of topological hierarchy insulator. To make it clear, we consider the Haldane model with a square-VSL and the lattice constant \( L \) set to \( 3a \). See the illustration in fig. 2(a). From the above discussion, there exists a \( \pi \)-flux in each square plaquette of VSL and a \( \frac{\pi}{2} \)-flux in each triangular plaquette of VSL. From the configuration of zero modes around vacancies in fig. 2(b), one can see that quantum states induced by VSL can be regarded as a new generation of lattice model, of which the vacancies play the role of the “atoms”.

As a result, we obtain an effective Hamiltonian that describes the vacancy-induced square lattice, written in the form

\[
\hat{H}_{L-VL} = -T \sum_{R \in A} (\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + i\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + \text{h.c.}) \\
+ T \sum_{R \in B} (\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R - i\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + \text{h.c.}) \\
+ T' \sum_{i \in A} (\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + \tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + \text{h.c.}) \\
- T' \sum_{i \in B} (\tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + \tilde{\hat{d}}_{R+Lx, Ly}^\dagger \tilde{\hat{d}}_R + \text{h.c.}),
\]

where \( T, T' \) are the effective NN and NNN hopping parameters, respectively. \( A \) and \( B \) label the sublattices of VSL. By comparing eq. (1) and eq. (6), one can see the corresponding relationship, \( \tilde{\hat{c}}_i \leftrightarrow \tilde{\hat{d}}_R \), \( t \leftrightarrow T \), and \( t' \leftrightarrow -T' \). For the defect-induced quantum states, the energy spectrum and DOS are obviously similar to those of the parent Hamiltonian in eq. (1).

From the DOS of the Haldane model with square-VSL for \( t'/t = 0.2 \) and \( L = 3a \) in fig. 2(c), the mid-gap energy bands appear near the chemical potential. It is obvious that the MG states are VSL induced. In particular, we found that the mid-gap states also have an energy gap and two points exist with van Hove singularity. The DOS of the MG states is very similar to that of the parent TBI (see the DOS of the parent TBI in fig. 1(b)). By fitting a curve to the DOS of the vacancy-induced quantum states, we obtain the effective hopping parameters as \( T = 0.22t \) and \( T' = 0.07t \).

Next, we will show that the MG states induced by VSL have similar topological properties to those of the parent TBI. By a numerical approach, we found that the Chern number of the MG states is \( C_{L-VL} = -1 \) contrary to that of the parent TBI

\[
C_{L-VL} = -C_{\text{parent}}.
\]

To characterize the Haldane model with square-VSL, we introduce the filling factor \( \nu = N_f/N \), where \( N \) is the total number of lattice sites and \( N_f \) is the number of fermions. The composite system is an insulator at filling factor \( \nu = \frac{1}{2} \) or \( \nu = \frac{1}{2}(1 - \frac{a^2}{2\pi}) \). At half-filling (or \( \nu = \frac{1}{2} \)), the total Chern number of the system is zero due to

\[
C_{\text{total}} = C_{\text{itinerant}} + C_{L-VL};
\]

at filling factor \( \frac{1}{2}(1 - \frac{a^2}{2\pi}) \), the total Chern number of the system is 1 due to

\[
C_{\text{total}} = C_{\text{itinerant}} = C_{\text{parent}}.
\]
Here $C_{\text{itinerant}}$ is the Chern number for itinerant electronic states that is equal to the Chern number of the parent topological insulator\(^1\).

To illustrate the topological properties of the Haldane model with square-VSL, we then studied its edge states. On the one hand, at the filling factor $\nu = 1$, the system becomes a TBI with Chern number 1. As a result, when the system has a periodic boundary condition along the $y$-direction but an open boundary condition along the $x$-direction, there exist gapless edge states. On the other hand, we consider the half-filling case, whose system has zero Chern number. However, the system still has nontrivial topological properties. When the parent topological insulator has a periodic boundary condition along both the $x$-direction and the $y$-direction, while the VSL has periodic boundary condition along $y$-direction but open boundary condition along $x$-direction, there may exist gapless edge states. See the numerical results in fig. 2(d) for the case of $t'/t = 0.2$ and $L = 3a$. We can see that there indeed exist gapless edge states on the boundaries of VSL.

In general, the Haldane model with a square-VSL of odd number $L^2$ has nontrivial topological properties and is different from traditional TBIs. As a result, we call this type of PH symmetry-protected TBI with topological MG states topological hierarchy insulator. In other words, THI is given by the following equation:

$$\text{THI} = \text{PH symmetry-protected TBI} + L \times L \text{ square-VSL} = \text{Parent TBI + topological MG states.}$$  (10)

\(^{1}\)For a TBI with dilute impurities, the Chern number will be not changed without gap-closing. Here, we consider a lattice of impurities (that are vacancies) and the distance between two impurities is large (or $\xi < L$). For this case, the itinerant electronic states of a TBI with VSL can be adiabatically changed from those without VSL. As a result, we believe that the Chern number for itinerant electronic states in a TBI with VSL is equal to the Chern number of electronic states in parent TBI without VSL.

To construct a TFI, we first consider a THI with self-similar MG states. Because we can tune $T'/T$ (or $\Delta E'/\Delta E$) by changing the NNN hopping parameter $t'$ of the parent TBI or the VSL constant $L$, the MG states can be self-similar to the parent topological states for the case of $T/T' = t'/t$. From numerical calculations, we obtain the self-similarity in the phase diagram of fig. 3(b), where smaller/bigger $t'/t$ leads to bigger/smaller $T/T'$. Now, under the self-similar condition $T/T' = t'/t'$, the effective Hamiltonian that describes the MG states becomes

$$\hat{H}_{1\text{-VL}} = \alpha \hat{H}_{\text{parent}}^*, \quad (11)$$

where $\alpha = T/t$ ($\alpha < 1$) is an energy-scaling ratio.

Next, we regard the vacancy-induced MG states as a parent TBI and introduce an additional VSL on it. Using the recursive relation, we can see that there exist additional MG states inside the energy gap of first-generation MG states (which we refer to as generation-1 MG states). Consequently, we obtain a new generation of topological MG states (we call such MG states in the energy gap of MG states as generation-2 MG states). Using the same procedure, we can construct a THI with $n$-generation MG states and eventually a THI with infinite generations of self-similar MG states that is just a TFI. Then, under the self-similar condition $T/T' = t'/t'$, the effective Hamiltonian of the generation-$n$ MG states is given by

$$\hat{H}_{n\text{-VL}} = \begin{cases} \alpha^n \hat{H}_{\text{parent}}^*, & \text{if } n \text{ is an even number}, \\ \alpha^n \hat{H}_{\text{parent}}^*, & \text{if } n \text{ is an odd number}. \end{cases} \quad (12)$$

From the DOS in fig. 3(c), we can see that the DOS of the MG states is always self-similar.

In addition, we discuss the Chern number of the TFI. The TFI is an insulator at filling factor $\nu = \frac{1}{2}(1 - \frac{2m}{L^2})$ where $m$ is an integer number, $m \geq 1$. The Chern number of generation-$m$ MG states is known to be

$$C_{m\text{-VL}} = (-1)^m. \quad (13)$$

As a result, at filling factor $\nu = \frac{1}{2}(1 - \frac{2m}{L^2})$, the total Chern number of the system is

$$C_{\text{total}} = C_{\text{itinerant}} + \sum_{n=1}^{m-1} C_{n\text{-VL}} = [1 + (-1)^{m-1}]/2. \quad (14)$$

For example, when the filling factor is $\frac{1}{2}(1 - \frac{2}{3})$ ($m = 3$), the total Chern number of the system is 1 due to

$$C_{\text{total}} = C_{\text{itinerant}} + C_{1\text{-VL}} + C_{2\text{-VL}}. \quad (15)$$

It is known that a self-similar object looks “roughly” the same on different scales and a fractal is a particularly self-similar object that exhibits a repeating pattern displaying at every scale. The topological fractal insulator provides a unique example of topological matters with self-similarity, in which the topological properties always look the same on different energy scales ($\alpha^{2n}$) or different length scales ($L^{2n}$).
Topological hierarchy insulators on a honeycomb lattice. – We finally study the THI based on the Haldane model on a honeycomb lattice, whose Hamiltonian is given by

$$\hat{H}_{\text{parent}} = -t \sum_{\langle i,j \rangle} \hat{c}_i \hat{c}_j - t' \sum_{\langle\langle i,j \rangle\rangle} e^{i\phi_{ij}} \hat{c}_i \hat{c}_j - \mu \sum_i \hat{c}_i \hat{c}_i^\dagger, \quad (16)$$

where $\hat{c}_i$ represents the fermion annihilation operator at site $i$. $t$ and $t'$ are the nearest-neighbor (NN) and the next-nearest-neighbor (NNN) hopping parameters, respectively. $e^{i\phi_{ij}}$ is a complex phase along the NNN link, and we set the direction of the positive phase clockwise ($|\phi_{ij}| = \pi$). $\mu$ is the chemical potential. The Haldane model on honeycomb lattice is also a Chern insulator with nonzero Chern number, $C_{\text{parent}} = 1$. The energy gap of the Haldane model on a honeycomb lattice is $\Delta_f = 6\nu/3't$ and the DOS is depicted in fig. 4(a).

Since the Haldane model of eq. (16) also satisfies the PH symmetry [15], $\hat{H}_{\text{parent}} = -P^T \hat{H}_{\text{parent}} P$, a vacancy also induces a fermionic zero mode and the particle density distribution around the vacancy is given in fig. 4(b). The particle density is also localized around the vacancy center within a length-scale $\sim (\Delta_f)^{-1}$. In the following, we focus on the Haldane model with a honeycomb-VSL shown in fig. 5(a), whose shortest distance $L$ between two vacancies is $5a$. The corresponding particle density distribution of fermionic zero modes induced by VSL is shown in fig. 5(b).

Due to the localized electronic states, each vacancy can be regarded as an isolated “atom”. Using a similar approach, we derive an effective Hamiltonian to describe the honeycomb-VSL

$$\hat{H}_{\text{L-VL}} = -T \sum_{\langle I,J \rangle} \hat{d}_I \hat{d}_J - T' \sum_{\langle\langle I,J \rangle\rangle} e^{i\phi_{IJ}} \hat{d}_I \hat{d}_J - \mu \sum_I \hat{d}_I \hat{d}_I^\dagger, \quad (17)$$

where $T$, $T'$ are the effective NN and NNN hopping parameters, respectively. $I$, $J$ denote the positions of vacancies. By comparing eq. (16) and eq. (17), one can see the corresponding relationship $\hat{c}_i \rightarrow \hat{d}_I$, $t \rightarrow T$, $t' \rightarrow T'$, $\phi_{ij} \rightarrow -\phi_{IJ}$.

The THI is an insulator at filling factor $\nu = 1/2$ or $\nu = \frac{24}{25}$. At half-filling (or $\nu = 1/2$), the total Chern number of the system is zero; at filling factor $\nu = \frac{24}{25}$, the total Chern number of the system is 1. In addition, we study the edge states of the MG states. See the numerical results in fig. 5(d) which exhibits its topological properties for the half-filling case. For a THI with $n$-generation MG states, the total Chern number of the system at filling factor $\nu = \frac{1}{2}(1 - \frac{24}{25})$ is $C_{\text{total}} = |1 + (-1)^{n+1}|/2$.

Discussion and conclusion. – In this paper, based on the Haldane model on a square lattice and on a honeycomb lattice, we studied the Chern insulators with VSL and found that the vacancy-induced MG states have nontrivial topological properties. We discovered new types of TBI—THIs and TFIs. These topological insulators are protected by a particle-hole symmetry. In particular, TFIs provide a unique example of topological matters with self-similarity, in which the topological properties always look the same on different energy scales. As a result, these exotic properties of THIs and TFIs will deepen our understanding of symmetry-protected topological states and provide additional possibility to design a complex dissipative electricity structure. In the future, similar topological states (THIs or TFIs) can be explored on other lattices (such as the triangle lattice or the kagome lattice).

Finally, we address the relevant experimental realizations of THI. In condensed-matter physics, one possible
realization is constituted by two-dimensional organic topo-
logical insulators made of organometallic lattices that
are designed by assembling molecular building blocks of
triphenyl-metal compounds with strong spin-orbit cou-
pling into a hexagonal lattice. This system has particle-
hole symmetry and can be considered as the possible can-
didate framework of topological hierarchy insulators and
topological fractal insulators [19]. On the other hand, ex-
perimental realizations of quantum many-body systems in
optical lattices have led to a chance to simulate a variety
of topological states. Recently, in ref. [20], the (spinless)
Haldane model on a honeycomb optical lattice has been
simulated in cold atoms. Because the VSLs on an opti-
cal honeycomb lattice can be achieved by using the holo-
graphic 2D arrays of microtraps with a given geometry,
THI may be realized on an optical lattice by using timely
cold-atom technology [21]. On the contrary, it is difficult
to realize THIs and TFIs based on the Haldane model on
a square lattice.

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