Supplemental material to the article

A new type of massless Dirac fermions in a crystalline topological insulators

Crystalline and crystalline topological insulators Quasiparticle dispersion law at symmetrical points in Brillouin (BZ) zone in the non-magnetic 1D, 2D and 3D structures is dictated by the space group symmetry of the crystal and the time-reversal invariance.

There are 230 three-dimensional (3D) crystal groups [1]. The electronic spectrum $\varepsilon_i(k_x, k_y, k_z)$ (i is band index) is determined by the irreducible representations of these groups. A cleaving three-dimensional (3D) infinite crystal into two semi-infinite crystal with the surface may lead to appearance of localized surface states on 3D crystal surface. The appearance or absence of such surface states is determined by the details of the Hamiltonian on the surface. The dispersion relation of the surface states $\varepsilon_i(k_x, k_y)$ in 3D a semi-infinite crystals is described by the irreducible representations of 17 2D surface groups [1].

Note that the surface states of a purely two-dimensional (2D) systems, such as monoatomic layer of graphite (graphene), are described by irreducible representations of the same 17 2D surface groups. The only difference is that in the semi-infinite crystal there is additional continuous spectrum, formed by the projections of Π_{k_z} bulk spectrum of the crystal – $\varepsilon_{i\ bulk}(k_x, k_y) = \Pi_{k_z}\varepsilon_{i\ bulk}(k_x, k_y, k_z)$ (situation 3D→2D).

In the case of a purely two-dimensional 2D systems projection of the bulk spectrum are absence, and there are only two-dimensional spectrum – $\varepsilon_i(k_x, k_y)$, the form of which is also determined by representations of one of the 17 2D surface groups.

A similar situation occurs for 2D crystals with a surface (2D→1D situation). Suppose there is an infinite 2D crystal, from which one can get a semi-infinite 2D system (2D system with 1D surface), or tape. On the surface of a semi-infinite 2D crystal or on the belt edge, can also occur surface (edge) states with one-dimensional dispersion $\varepsilon_i(k_x)$. From the point of view of the symmetry the dispersion of surface states in a semi-infinite 2D crystal or tape, should be described by the representations of one of the 7 crystal 1D groups (groups of borders [1]).

When you cut a semi-infinite crystal (or tape) from the 2D system, the spectrum of an infinite 2D crystal $\varepsilon_{ibulk}(k_x) = \Pi_{k_y}\varepsilon_{ibulk}(k_y, k_x)$ (2D→1D) projected onto the surface and forms 1D, as in the previous case – 3D→2D, projection bulk bands. Surface (edge) states with one-dimensional $\varepsilon_i(k_x)$ dispersion, if they do not fall into the projection of bulk bands to be classified according to the irreducible representations of one of the seven groups of 1D crystal borders.

Further, when the 2D or 3D volume range is as follows. that the system is an insulator, the projections of different bulk bands do not overlap at any points in k-space (k_x, k_y in 2D, and at k_x 1D), then the system without surface states is an insulator. It is assumed that the number of electrons per unit cell such that the Fermi level is in the bulk energy gap.

However, if in the projections of the bulk energy gap surface states arise and intersect the Fermi level, then the system becomes conductive on the surface (metal or semimetal – this is the detail of terminology) while remaining insulator in the bulk.

- For a listing of all the types of features of the spectrum of surface states at the symmetry points in the Brillouin zone in 3D→2D, a 2D→1D and 2D purely two-dimensional cases, no topological argument is not required. One needs only to spatial representations of the corresponding crystalline groups and invariance under time reversal.

- The presence of surface states, their position in energy relative to the projections of a bulk bands in the 3D→2D and 2D→1D cases determined by the details of the Hamiltonian on the surface.

Conical Dirac spectrum with greater than 2-fold degeneracy (up to 16-fold) occurs in field theories and superfluid ^{3}He-A (see, eg, [2] and references therein). However, the symmetry groups in these models, very different than the crystalline group whose views and dictate the appearance of these features. Presentation

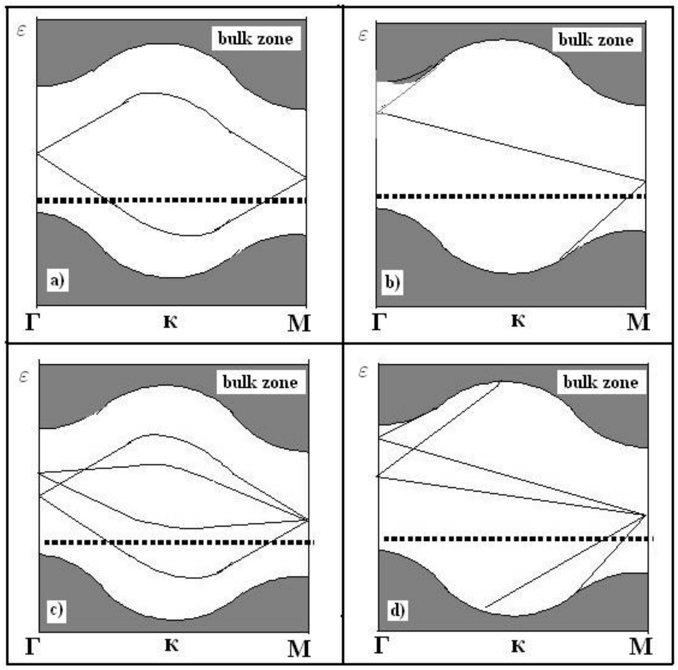

Figure 1: The projections of the bulk bands and surface states. Case 2-fold degeneracy: a) conventional insulator, b) a topological insulator. Case 4-fold degeneracy: c) conventional insulator, d) a topological insulator.

of a particular symmetry of the crystal system provides a recipe for the implementation of this spectrum through artificial structures with this symmetry. Moreover, there may be created with the desired photonic crystal symmetry, where there must be similar spectral features.

The methods of algebraic topology in this problem arise when one can try to answer the following question.

Suppose we have two Hamiltonian $\mathcal{H}_1$ and $\mathcal{H}_2$, describing the 3D→2D (or 2D→1D) system, each of which is invariant with respect to the crystal symmetry group and inversion time, and gives the surface states in the Brillouin zone symmetry points out projections of bulk bands. Hamiltonians are continuous deformation, which is achieved by varying the parameters describing them, the same way that the gap in projected bulk bands do not slam. Surface states are genetically derived from the states of bulk bands and the total number of states in the crystal does not change, then there are two possible situations.

In the first situation (Fig. 1 b).d))), the deformation of $\mathcal{H}_1$, surface states may be forced out of the band gap of the projections of the spectrum to the continuum (the projection of bulk bands). The system would be an insulator as in the bulk and on the surface. Systems with Hamiltonians of this type are called conventional insulators.

In the second case (Figure 1a),c)), the deformation of $\mathcal{H}_2$ can not push out of the surface states to continuous spectrum (bulk bands). The system is an insulator in volume, but remains metal on the surface. Systems with such Hamiltonians are called topological insulators.[1]

The whole set of Hamiltonians satisfying the requirements of the crystal symmetry and time reversal, considered as a topological manifold is divided into equivalence classes. To characterize these classes are convenient topological invariants which do not depend on the particular Hamiltonian, and depend only on the equivalence class. If the two Hamiltonians have different topological invariants, then obviously they belong to different classes.

The choice is dictated by a set of invariants of a physical challenge, and the fact that there should be a constructive procedure for computing invariants on the basis of diversity, such as Hamiltonians. The goal of topological analysis is to break the variety of Hamiltonians into equivalence classes, distinguishing topological

[1] Traditionally topological insulators in the case of 3D→2D called 3D, as in the case of 2D→1D 2D, or more often, the spin-Hall topological insulators [5, 6], which can lead sometimes to confusion.

insulators from conventional insulators.

Topological classification is as follows (see [3]). It is assumed that there exist surface states. It is constructed the Hamiltonian $\mathcal{H}$ ($\mathbf{k}$), describing the surface states for a given crystal group (here $\mathbf{k}= (k_x, k_y)$ for the 3D→2D, and $\mathbf{k}= (k_x)$ for the 2D→1D cases).

Since the wave function is an eigenfunction of the Hamiltonian for the calculation of topological invariants need to know the behavior of the wave functions for the entire Brillouin zone, it is necessary to have a complete the Hamiltonian $\mathcal{H}(\mathbf{k})$, which takes into account all the features of the spectrum of surface states dictated symmetry. In actual calculations, the Hamiltonian is written in the tight-binding (with hoppings in the lattice between nearest neighbors or next-nearest, [3]). After that starts the Hamiltonian depends explicitly on a set of model parameters $\{d\}$ – $\mathcal{H}$ ($\mathbf{k}$, $\{d\}$).

For a listing of different equivalence classes of Hamiltonians (topological phases) is used, so-called, $\mathcal{Z}_2$ classification [3–5]. Since all of the wave function are $|\psi_{i,\mathbf{k}}\rangle$ (i – band index) eigenfunctions of $\mathcal{H}(\mathbf{k}$, $\{d\})$, then the functions of different itinerant indexes represent different branches of a single function, defined on the Riemann surface. This allows you to enter a single function for the entire Brillouin zone for different values of $\mathbf{k}$. Let $\mathcal{K}$ – time reversal operator. Since the Hamiltonian is invariant under time reversal, the spectrum is also invariant under the inversion pulse quasi-momentum ($\varepsilon(\mathbf{k}) = \varepsilon(-\mathbf{k})$), with the branches of the spectrum with $\mathbf{k}$ and $-\mathbf{k}$ functions can meet with one or a few sheets of the Riemann surface. This information is included in the value of a polynomial – the Pfaffian of a skew-symmetric matrix formed from the elements of $\langle\psi_{j,\textbf{-k}}|\mathcal{K}\psi_{i,\mathbf{k}}\rangle$. The value of the polynomial (Pfaffian), because the total wave function on the Riemann surface is a topological invariant, whose value is dependent at BZ $\mathbf{k}$ and a set of parameters $\{d\}$, describing the Hamiltonian $\mathcal{H}(\mathbf{k}$,$\{d\})$. Convenient to use the normalized value [3–5]

$$\delta(\mathbf{k}, \{d\}) = \sqrt{\mathrm{Det}\{\langle\psi_{j,\textbf{-k}}|\mathcal{K}\psi_{i,\mathbf{k}}\rangle\}}/\mathrm{Pf}\{\langle\psi_{j,\textbf{-k}}|\mathcal{K}\psi_{i,\mathbf{k}}\rangle\},$$

where as the $\mathbf{k}$ – vector is taken in a symmetric point Brillouin zone for the case of one-dimensional 2D→1D, and for the case of two-dimensional 3D →2D (see [3]).

In the symmetric points of the BZ $\mathbf{k}$ and **-k** are not only time-reversal operation, but also the elements of symmetry of the crystal. The value of $\delta(\mathbf{k}, \{d\})$, which is a topological invariant, can be set to $\pm$ 1 and can be expressed explicitly (when fixing the symmetrical point in the BZ) through the parameters of the Hamiltonian $\mathcal{H}(\mathbf{k}$,$\{d\})$, defined over the entire BZ. Different sets of values ($\delta(\mathbf{k}_{isym}, \{d\})$ symmetric points $\mathbf{k}_{isym}$, depending on the set $\{d\}$, describe the different equivalence classes (the topological phase) Hamiltonians $\mathcal{H}(\mathbf{k}$,$\{d\})$.

Possible topological phases and their classification for the surface states is determined by a set of parameters of the Hamiltonian for these states.

Informal meaning of the topological invariant [3] is as follows. In the case, 2D→1D Hamiltonian is $\mathcal{H}(\mathbf{k},\{d\})(\mathbf{k} = k_x)$, and the surface BZ is a segment. Dirac cone is only possible in the center of the zone and at the border. In this case, the invariant gives the number of intersections ($\delta = +1$ – even, $\delta = -1$ – odd) surface states of the Fermi level. Different values of the topological invariant correspond to different ways of transition between the branches of the spectrum of surface states at different points in the Brillouin zone (Fig. 1). In a case of an even number of crossings (Fig. 1), the surface states can be stamped in the projection of bulk bands. When an odd number of intersections (Fig. 1), the surface states can not be pushed out of the band gap and are in this sense are topologically protected. In a formal language the number of intersections of the Fermi level is the number of transitions from one sheet of the Riemann surface on the other when the quasi-momentum from one point to another symmetrical point. Have a similar meaning invariants for 3D→2D situation. In this case, there is a set of topological invariants for symmetric points, each of which has a sense of the number of crossings of the Fermi level in the motion along the line coupling of points with $\mathbf{k}$ and $-\mathbf{k}$. A set of invariants for symmetric points characterizes a particular topological phase.

In the case of 2-fold degeneracy of the Dirac cone as possible in the center of the Brillouin zone (point of Γ), and in the edge of the BZ M point. Surface states are topologically stable in the sense that it cannot be of pushed to bulk bands only if *odd* number of intersections of the Fermi level (Fig. 1b)). If *even* the number of crossings - surface states are unstable (Figure 1a)) and can be pushed out of the band gap. Is therefore sufficient to $\mathcal{Z}_2$ classification.

In the case of the 4-fold degeneracy at the point M we have a different situation. At the point of Γ is allowed only 2-fold degeneracy. Even with the *even* the number of intersections of the Fermi level (Fig. 1) may be unsustainable (ris.2c)) and stable surface states (Fig. 1d)), which may require a *a different set of topological invariants.*

The fundamental point to understand the situation is as follows. By itself does not give a topological classification of the types of singularities of the electronic spectrum, 2-fold degenerate, 4-fold degenerate Dirac cones and others mentioned above features. *These features are dictated by the crystal symmetry in conjunction with the operation of time reversal, and laid in the Hamiltonian of the "hands". Topological invariants only way to fix the connection features of the spectrum, which are incorporated in the Hamiltonian, and can not predict the features themselves.* Therefore, if the form of the Hamiltonian does not take into account all the possible features of the spectrum dictated by the crystal symmetry and the inverse of the time, part of the topological phases (different set of values $(\delta(\mathbf{k}_{isym}, \{d\}))$, will be skipped. For a listing of all the features needed tppov themselves other than the topological invariants, mathematical tools.

Symmetry allows for 4-fold degenerate Dirac cones that are not in full, according to the authors of [5], the topological classification. Such features are not played by the Hamiltonian used in [5]. In this you can see directly as a model Hamiltonian $\mathcal{H}(\mathbf{k},\{d\})((\mathbf{k} = (k_x, k_y)$ [5] does not contain the Dirac features more than 2-fold degeneracy. Therefore, the topological classification, based on a calculation of $\mathcal{Z}_2$ invariants in [5], is not complete.

The Hamiltonian in [5] is taken in the form.

$$\hat{\mathcal{H}}(\mathbf{k}) = \begin{pmatrix} \mathcal{H}(\mathbf{k}) & 0 \\ 0 & \mathcal{H}(\text{-}\mathbf{k}) \end{pmatrix},$$

$\mathcal{H}(\mathbf{k})$ and $\mathcal{H}(\text{-}\mathbf{k})$ – correspond to points related to the inverse of the time in the lattice. In the case of a point M, all points of M are equivalent, and the Hamiltonian in [5] is - $\mathcal{H}(\mathbf{k}) \sim \sigma \cdot \mathbf{d}(\mathbf{k})$($\sigma$ – vector of the Pauli matrices). The spectrum at a point M has the form $\varepsilon(\mathbf{k}) \sim \pm|\mathbf{d}(\mathbf{k})|$ $(\mathbf{k} = (k_x, k_y))$, which implies that the spectrum at M has only a 2-fold degeneracy, rather than 4-fold degeneracy.

The Hamiltonian $\mathcal{H}$ $(\mathbf{k}, \{d\})$ $(\mathbf{k} = (k_x, k_y)$ should be parameterized throughout the two-dimensional Brillouin zone in such a way as to reproduce all allowable range of features in symmetrical points. Above were clearly facing new, not previously discussed for topological insulators, 4-fold degenerate Dirac cone that can exist at a point M in the two-dimensional Brillouin zone. In the center of the Brillouin zone in the point Γ is only possible 2-fold degenerate Dirac cone. Feature in the spectrum with a greater degree of degeneracy symmetry is not allowed. More than obvious that this type of features will lead to new topological phases (sets of values of topological invariants of $\delta(\mathbf{k}_{isym}, \{d\})$, where possible new ways of connecting singular points of the spectrum of surface states.

Knowing all types of features can be parameterized $\mathcal{H}$ $(\mathbf{k}, \{d\})$ $(\mathbf{k} = (k_x, k_y)$ for the whole Brillouin zone, so that reproduced all the features of the spectrum in the symmetric points, then calculate invariants is a purely technical problem. Because in itself it requires additional space, it makes sense to bring these results separately.

References

[1] B.K.Vainstein, *Crystallography*, v. Nauka, Moscow, (1979) (in Russian).

[2] G.E.Volovik, arXiv/cond-mat/0601372.

[3] M.Z.Hasan, C.L.Kane, Rev. Mod. Phys., **82** 3045 (2010).

[4] Xiao-Liang Qi, Shou-Cheng Zhang, Rev. Mod. Phys., **83** 1057 (2011).

[5] R.-J.Slager, A.Mesaros, V.Juriycic, J.Zaanen, *The space group classification of topological band-insulators*, Nature Phys., **9**, 98 (2013).