Supplemental material to the article

On the symmetrical-topological classification of edge states in crystalline spin Hall insulators with inversion time

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A comparison with other topological classifications.

One classification of edge states in 2D→1D systems based on the properties of the Pfaffian, introduced in [1] and is widely used in subsequent studies (see [1] and references in [2]). The argument is based on the so-called, bulk-boundary correspondence. Let there be a 2D→1D system. Let $|u_m(\mathbf{k})\rangle$ Bloch functions *of 2D system.* Operation time reversal $\mathcal{K}$ translates the state $|u_m(\mathbf{k})\rangle$ in the state $\mathcal{K}|u_m(\mathbf{k})\rangle$ with the opposite value of the momentum $-\mathbf{k}$. The bulk 2D Brillouin zone has two pairs of symmetric points $\mathbf{k}_a$ ($a = 1,2$) and $-\mathbf{k}_a$ ($a =$ 3,4), which are projected in the surface 1D Brillouin zone, respectively, Γ and X. Construct a matrix with the elements on the *bulk* Bloch functions $w_{nm}(\mathbf{k}) = \langle u_n(\mathbf{k})|\mathcal{K}|u_m(-\mathbf{k})\rangle$ ($n, m = 1, 2$ - band indices). Because of the anti-unitary $\mathcal{K}$ matrix $w_{nm}(\mathbf{k})$ is antisymmetric. The determinant of an antisymmetric 2×2 matrix $w_{nm}(\mathbf{k})$ is by definition the square of its Pfaffian

$$\delta_i = \mathrm{Pf}\{w_{nm}(\mathbf{k}_i)\}/\sqrt{\mathrm{Det}\{w_{nm}(\mathbf{k}_i)\}} = \pm 1, \tag{1}$$

where $\mathbf{k}_i \to \Gamma, X$. And the value of $|\langle u_1(\mathbf{k})|\mathcal{K}|u_2(-\mathbf{k})\rangle| = |P(\mathbf{k})| = 1$ (for real values of $\mathbf{k}$), if the function $|u_1(\mathbf{k})\rangle$ and $\mathcal{K}|u_2(\mathbf{k})\rangle$ is linearly dependent, and $|P(\mathbf{k})| = 0$ if $|u_1(\mathbf{k})\rangle$ and $\mathcal{K}|u_2(\mathbf{k})\rangle$ is linearly independent.

A topological invariant ν is defined as

$$(-1)^\nu = \prod_{a=1}^{4} \delta_a, \tag{2}$$

because $\delta_i = \pm 1$, then it is concluded that the types of surface states can be divided into two equivalence classes ($\mathcal{Z}_2$ classification). Even the value of ν corresponds ordinary insulator, odd value ν - topological insulator. This means that the surface states, if they exist in the gap, in a system with $\nu \bmod 2 = 0$, they are topologically unstable - can be removed from the gap to a projections of bulk bands. At $\nu \bmod 2 = 1$ surface states are topologically stable (topologically protected) and can not be pushed out of the gap by a continuous deformation of the Hamiltonian. As an illustration, in some papes presents calculations of the topological invariant for the model Hamiltonian in the tight-binding method, but *for a system with real border - tapes.*

In our view, this classification of types of surface states contains some logical inconsistencies.

1) In the construction of a topological invariant is used it the wave function of the volume of the Hamiltonian of the infinite 2D crystal without surface (border). However, the bulk Hamiltonian (see the discussion above in the main text) does not contain surface states. Therefore, the assertion that the sign of the invariant (1,2) gives a classification of insulators into two types - conventional and topological is not clear.

2) One would think that the Pfaffian method classifies topologically different types of bulk 2D Hamiltonians Pfaffian method even for the bulk states of catches in the inversion time, apparently, the union of one-dimensional representations. For example, in the case where the function $|u_m(\mathbf{k})\rangle$ and $\mathcal{K}|u_n(\mathbf{k})\rangle$ are linearly dependent, then according to this classification, the system does not can be topologically stable

states at the surface (topologicaly protected states), since $|\langle u_1(\mathbf{k})|\mathcal{K}|u_2(-\mathbf{k})\rangle| = |P(\mathbf{k})| = 1$, and so the system is known to be an ordinary insulator.

Counterexample is the following. If the functions $|u_m(\mathbf{k})\rangle$ and $\mathcal{K}|u_n(\mathbf{k})\rangle$ are the basic functions which belong to the same two-dimensional irreducible representation, then they are linearly dependent (this case relates to the a_1 Herring on [3,4] (see details in [3])), such a situation takes place in groups (p2mm) and (p2gm)) at the points of Γ and X. Spectrum in this situation is also conical (see the table in the main text). Therefore, even if $|\langle u_1(\mathbf{k})|\mathcal{K}|u_2(-\mathbf{k})\rangle| = |P(\mathbf{k})| = 1$ the system can be both conventional or topological insulators depending on the behavior of $\{a^i(k)\}$ over the entire Brillouin zone - ways to connect branches of the spectrum in Γ and X (Figure 1a) b) in the main text). This fact is a clear indication of the fact that $\mathcal{Z}_2$ classification based on *analytic properties of the Pfaffian near a singular point in the spectrum*, contains the logical inconsistencies in the identification of equivalence classes of surface states in the 2D→1D systems.

3) Finally, the third objection to the construction of topological invariants, based on the volume of Hamiltonians.

In 17 two-dimensional space groups there is one 2D space nonsymorphic group with glide planes (group 12, see [6]), which contains, at M points - edges of the two-dimensional Brillouin zone, a 4-fold force-degenerate, due to space symmetry and time reversal, conic spectrum. This 4-fold degenerate conic spectrum survives in the case of projecting it to the one-dimensional Brillouin zone. However, the systematics of the spectrum in a 2D system *with a boundary* is subject to classification for 7 groups of semi-infinite crystal (2D→1D systems). In these systems, let alone 2-fold degenerate conic spectrum in the Γ and X points. Therefore, in this case the topological invariant (1,2), calculated using the bulk 2D functions will have no relationship to the surface states at the border.

Despite the fact that the topological classification is based on the Pfaffian is used in many studies (references in [2]), it does not mean that the nature of the stability of the topological surface states fully understood.

References

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