Lecture notes on topological insulators

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(Dated: March 7, 2017)

I. POINT DEGENERACY BETWEEN ENERGY BANDS

The topology of an energy band is protected by an energy gap. It can change only if the gap is closed. We now study the criterion of having such a topological phase transition. The discussion is mainly based on Murakami's analysis (Murakami, 2008a,b).

A. Crossing between two levels

We start with the simpler, two-level case. The Hamiltonian can be expanded by the Pauli matrices,

$$\mathsf{H} = d_0(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}. \tag{1.1}$$

This gives the energy spectrum,

$$E_\pm = d_0 \pm \sqrt{d_x^2 + d_y^2 + d_z^2}. \tag{1.2}$$

An accidental degeneracy occurs only when $d_x = d_y = d_z = 0$. That is, one needs to tune 3 parameters to have a point degeneracy (see Fig. 1). We say that the degeneracy has **co-dimension** 3. This is first pointed out by von Neumann and Wigner (1929).

As a result, in 2D, it's unlikely to have an accidental degeneracy unless, in addition to (k_x, k_y), one can vary the third parameter. On the other hand, in a 3D BZ, one can expect to see isolated accidental degeneracies.

The nodal points in graphene cannot be considered as accidental, since they are protected by symmetries. Under time reversal and space inversion ($\Pi = \sigma_x$), one has (ignoring spin)

$$\text{TR}: \quad \mathsf{H}^*(\mathbf{k}) = \mathsf{H}(-\mathbf{k}), \tag{1.3}$$
$$\text{SI}: \quad \sigma_x \mathsf{H}(\mathbf{k}) \sigma_x = \mathsf{H}(-\mathbf{k}). \tag{1.4}$$

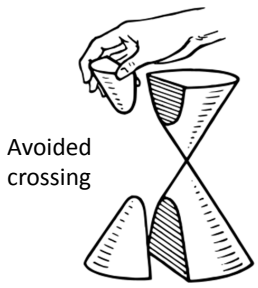

FIG. 1 Two levels could have isolated point degeneracies in 3D parameter space. Therefore, when one varies only one or two parameters, it is likely to miss the target and get an avoided crossing (Fig. is from Wikipedia)

TABLE I Clifford matrices and their symmetries

Γ	$\Theta\Gamma\Theta^{-1}$	$\Pi\Gamma\Pi^{-1}$
$\Gamma_0 = 1 \otimes 1$	$+$	$+$
$\Gamma_1 = \sigma_z \otimes \tau_x$	$-$	$-$
$\Gamma_2 = 1 \otimes \tau_y$	$-$	$-$
$\Gamma_3 = 1 \otimes \tau_z$	$+$	$+$
$\Gamma_4 = \sigma_x \otimes \tau_x$	$-$	$-$
$\Gamma_5 = \sigma_y \otimes \tau_x$	$-$	$-$
$\Gamma_{12} = \sigma_z \otimes \tau_z$	$-$	$+$
$\Gamma_{13} = -\sigma_z \otimes \tau_y$	$+$	$-$
$\Gamma_{14} = \sigma_y \otimes 1$	$-$	$+$
$\Gamma_{15} = \sigma_x \otimes 1$	$-$	$+$
$\Gamma_{23} = 1 \otimes \tau_x$	$+$	$-$
$\Gamma_{24} = -\sigma_x \otimes \tau_z$	$-$	$+$
$\Gamma_{25} = -\sigma_y \otimes \tau_z$	$-$	$+$
$\Gamma_{34} = -\sigma_x \otimes \tau_y$	$+$	$-$
$\Gamma_{35} = \sigma_y \otimes \tau_y$	$+$	$-$
$\Gamma_{45} = \sigma_z \otimes 1$	$-$	$+$

This leads to

$$(d_x(-\mathbf{k}), d_y(-\mathbf{k}), d_z(-\mathbf{k})) = (d_x(\mathbf{k}), -d_y(\mathbf{k}), d_z(\mathbf{k})), \tag{1.5}$$
$$(d_x(-\mathbf{k}), d_y(-\mathbf{k}), d_z(-\mathbf{k})) = (d_x(\mathbf{k}), -d_y(\mathbf{k}), -d_z(\mathbf{k})) \tag{1.6}$$

When both symmetries exist, the σ_z term is not allowed. So the co-dimension of the degeneracy reduces to 2, and it's likely to have point degeneracies in a 2D BZ. Furthermore, a small perturbation with only σ_x-term and σ_y-term (respecting both TRS and SIS) could not lift the point degeneracy. For more discussions, see Chap 7 of Bernevig and Hughes, 2013).

On the other hand, when a magnetic field is applied (breaking TRS), or when the sublattices are composed of different atoms (breaking SIS, as in BN, boron nitride), the nodal points are opened.

B. Crossing between four levels

As shown in Chap. **??**, the Hamiltonian of a 4-level system can be expanded by 16 Clifford matrices

$$\mathsf{H}(\mathbf{k}) = h_0(\mathbf{k}) + \sum_{a=1}^{5} h_a(\mathbf{k}) \Gamma_a + \sum_{ab} h_{ab}(\mathbf{k}) \Gamma_{ab}, \tag{1.7}$$

where all of the $h(\mathbf{k})$ functions are real.

If H has time-reversal symmetry, then according to Table. I (see Chap **??**), 6 of the $h(\mathbf{k})$'s need to be even, and 10 of the $h(\mathbf{k})$'s odd, functions of $\mathbf{k}$. They could all exist with proper parities, and the number of Clifford basis cannot be reduced by TRS alone.

1. Inversion symmetry

(a) If conduction band and valence band have the same parity, then the SI operator is

$$\Pi = 1 \otimes 1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{1.8}$$

As a result, all of the signs on the right column of Table **??** would be "+".

If the system has SIS, then all of the $h(\mathbf{k})$'s need be even functions. If the system has TRS, then 10 of the $h(\mathbf{k})$'s need be odd (see the discussion above). So with both symmetries, only 6 of the Clifford bases survive,

$$\mathsf{H} = \varepsilon_0 + h_3\Gamma_3 + h_{13}\Gamma_{13} + h_{23}\Gamma_{23} + h_{34}\Gamma_{34} + h_{35}\Gamma_{35}, \tag{1.9}$$

in which all of the $h(\mathbf{k})$'s are even functions of $\mathbf{k}$. According to Eqs. (**??**) in Chap. **??**, the anti-commutator of any two of these five Clifford matrices is zero. Therefore, the eigen-energies are

$$E(\mathbf{k})_\pm = \varepsilon_0(\mathbf{k}) \pm \sqrt{\sum_i h_i^2}, \tag{1.10}$$

where i runs over the 5 indices above.

First, the energy spectrum has global 2-fold degeneracy, as expected. Second, to close the energy gap, one needs to tune 5 parameters so that all 5 of the h_i's are zero. That is, the degenerate point has co-dimension 5. Therefore, varying the 3D momentum $\mathbf{k}$ and an extra parameter m is not enough to close the gap.

(b) On the other hand, if conduction band and valence band have opposite parity, then

$$\Pi = 1 \otimes \tau_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{1.11}$$

The right column of Table **??** shows the parities of the Clifford matrices under such a SI operator.

If the system has SIS, then half of the $h(\mathbf{k})$'s need be even, and the other half odd, functions of $\mathbf{k}$. If the system has TRS, then again 10 of the $h(\mathbf{k})$'s need be odd. So with both symmetries, only the first 6 Clifford bases without conflicting $h(\mathbf{k})$-parities could survive,

$$\mathsf{H} = \varepsilon_0 + \sum_{a=1}^{5} h_a \Gamma_a, \tag{1.12}$$

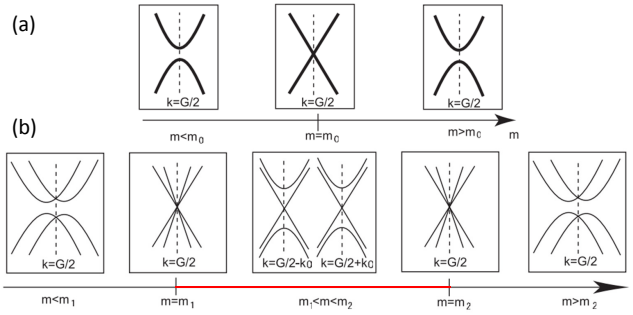

FIG. 2 (a) For a system with both TRS and SIS, if the conduction band and valence band have opposite parities, then one can close the gap at TRIM with one parameter m. (b) If the SIS of the system in (a) is broken, then the critical point m_c could be extended to an interval of gapless region, $m_1 \le m \le m_2$. (The figures are from Murakami, 2008a)

in which h_3 is even in $\mathbf{k}$, while $h_{1,2,4,5}$ are odd in $\mathbf{k}$. The eigen-energies are

$$E(\mathbf{k})_\pm = \varepsilon_0(\mathbf{k}) \pm \sqrt{\sum_{a=1}^{5} h_a^2}. \tag{1.13}$$

If $\mathbf{k}$ is not a TRIM at $\mathbf{G}/2$, then the co-dimension of the degeneracy is 5. However, if $\mathbf{k} = \mathbf{G}/2$, then $h_{1,2,4,5}(\mathbf{G}/2) = 0$. Therefore, at a TRIM, the co-dimension reduces to 1. That is, one only needs to tune one parameter m to kill h_3 and close the gap at TRIM (see Fig. 2(a)). This analysis applies to 2D as well.

The lesson is, to fabricate a point degeneracy, it's better to work with two energy bands with opposite parities.

2. Without inversion symmetry

If the system has only TRS, but no SIS, then even though there is Kramer degeneracy, the energy spectrum would not have global 2-fold degeneracy. With appropriate parameters, there might be 4-fold degeneracy at TRIM. Away from TRIM, it's unlikely to have the 4-level crossing, and therefore only 2 levels need be considered. As a result, we are back to the 2-level case,

$$\mathsf{H} = d_0(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}. \tag{1.14}$$

The co-dimension is 3. So for a 2D system, there could be isolated point degeneracies in the 3D $(\mathbf{k}, m)$-space. For a 3D system, there could be isolated point degeneracies in the 3D BZ, and a line of point degeneracy in the 4D $(\mathbf{k}, m)$-space (see Fig. 2(b)).

References

Bernevig, B. A., and T. L. Hughes, 2013, *Topological Insulators and Topological Superconductors* (Princeton University Press).

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Murakami, S., 2008b, Prog. Theo. Phys. Supplement **176**, 279.