Problem set 5 for "Topology in condensed matter"

To be discussed in exercise class on January 23, 2024

1 Bernevig-Hughes-Zhang model

In this problem you will study a specific example of a model with $\mathbb{Z}_2$ topological order. The 4×4 Hamiltonian in the momentum representation with the Brillouin zone $k_{x,y} \in [-\pi, \pi]$ has a block structure in the Kramers-partner space:

$$\hat{H}(\boldsymbol{k}) = \begin{pmatrix} \hat{h}(\boldsymbol{k}) & 0 \\ 0 & \hat{h}^*(-\boldsymbol{k}) \end{pmatrix}, \quad \hat{h}(\boldsymbol{k}) = \begin{pmatrix} \xi_{\boldsymbol{k}} & A(\sin k_x - i \sin k_y) \\ A(\sin k_x + i \sin k_y) & -\xi_{\boldsymbol{k}} \end{pmatrix} \tag{1}$$

with $\xi_{\boldsymbol{k}} = u - t(\cos k_x + \cos k_y)$, assuming $A, t > 0$ and arbitrary u.

1. Check that the Hamiltonian obeys time-reversal symmetry (TRS) $\mathcal{T} = i\hat{s}_y\mathcal{K}$ (with $\mathcal{K}$ being complex conjugation, and $\hat{s}_{x,y,z}$ being Pauli matrices acting in the Kramers-partner space):

   $$\mathcal{T}\hat{H}(\boldsymbol{k})\mathcal{T}^{-1} = \hat{H}(-\boldsymbol{k}). \tag{2}$$

   Show that $\hat{\mathcal{T}}^2 = -1$, so that Kramers' theorem holds and the system describes two double-degenerate bands, denoted as $E_\pm(\boldsymbol{k})$.

2. In addition to the TRS, shown that the Hamiltonian also obeys conventional unitary *inversion symmetry* $\mathcal{I} = \hat{\sigma}_z$ (with $\hat{\sigma}_{x,y,z}$ the Pauli matrices acting on the inner block structure), so that:

   $$\mathcal{I}\hat{H}(\boldsymbol{k})\mathcal{I}^{-1} = \hat{H}(-\boldsymbol{k}). \tag{3}$$

   As a consequence, the eigenstates of the Hamiltonian at *time-reversal symmetric points* of the Brillouin zone $\boldsymbol{\Lambda}_{1,2,3,4} = \{(0,0), (0,\pi), (\pi,0), (\pi,\pi)\}$ can be also classified by corresponding eigenvalues of the inversion operator $\zeta(\boldsymbol{\Lambda}_i) = \pm 1$. Calculate eigenvalues of the inversion operator for filled states and show that the $\mathbb{Z}_2$ topological index, defined for such systems as

   $$(-1)^\rho = \prod_{i=1}^{4} \zeta(\boldsymbol{\Lambda}_i) \tag{4}$$

   is nontrivial (i.e. $\rho = 1$) when $u \in [-2t, 2t]$.
   Hint: show that the Hamiltonian at $\boldsymbol{\Lambda}_i$ is itself proportional to the inversion operator $\hat{H}(\boldsymbol{\Lambda}_i) = g_i\hat{\mathcal{I}}$, and relate $\zeta(\boldsymbol{\Lambda}_i)$ to g_i.

3. Diagonalize the Hamiltonian and find its eigenvalues $E_\pm(\boldsymbol{k})$ and corresponding eigenvectors $|u(\boldsymbol{k})\rangle$. Calculate the matrix elements of the TR operator over the filled bands

   $$M_{ij}(\boldsymbol{k}) \equiv \langle u_i(\boldsymbol{k})| \mathcal{T} |u_j(\boldsymbol{k})\rangle . \tag{5}$$

   In general, the $\mathbb{Z}_2$ topological index can be deduced from the consideration of zeros of Pfaffian of the matrix $P(\boldsymbol{k}) = \mathrm{Pf} M(\boldsymbol{k})$ in *half* of the Brillouin zone. Show by explicit calculation that zeros of $P(\boldsymbol{k})$ appear only in the topological phase but along the lines in the momentum space and not at isolated points.

4. A more generic form of the Hamiltonian includes also off-diagonal elements:

   $$\hat{H}(\boldsymbol{k}) = \begin{pmatrix} \hat{h}(\boldsymbol{k}) & \hat{c}(\boldsymbol{k}) \\ \hat{c}^\dagger(\boldsymbol{k}) & \hat{h}^*(-\boldsymbol{k}) \end{pmatrix}. \tag{6}$$

   What conditions should matrix $\hat{c}(\boldsymbol{k})$ satisfy in order for the whole system to be time-reversal symmetric?

2 Classes A, AII and $AIII$ in 3D

Consider a two-dimensional surface of some three-dimensional material without particle-hole symmetry, which can host gapless states. Such Hamiltonian by construction should depend on two components of momenta, k_1 and k_2, and in the vicinity of the point where surface dispersion crosses the chemical potential (which we assume to be $\boldsymbol{k} = (0, 0)$ without loss of generality) should assume linear expansion of the form:

$$\hat{H}_{\text{surf}}(\boldsymbol{k}) = k_1 \hat{\gamma}_1 + k_2 \hat{\gamma}_2, \tag{7}$$

where γ_1 and γ_2 are 2×2 mutually anticommuting matrices. Moreover, without loss of generality, one can perform a continuous deformation of the Hamiltonian such that these matrices are $\hat{\gamma}_1 = \hat{\sigma}_x$ and $\hat{\gamma}_2 = \hat{\sigma}_y$ in some basis.

1. Show that this Hamiltonian obeys chiral symmetry $\hat{\mathcal{C}} \hat{H}_{\text{surf}}(\boldsymbol{k}) \hat{\mathcal{C}} = -\hat{H}_{\text{surf}}(\boldsymbol{k})$ with $\hat{\mathcal{C}}^2 = 1$, and time-reversal symmetry $\hat{\mathcal{T}} \hat{H}_{\text{surf}}(\boldsymbol{k}) \hat{\mathcal{T}}^{-1} = \hat{H}_{\text{surf}}(-\boldsymbol{k})$, where $\hat{\mathcal{T}} = \hat{U}_T \mathcal{K}$ with some unitary matrix $\hat{U}_T$ and complex conjugation $\mathcal{K}$. What are the matrices $\hat{\mathcal{C}}$ and $\hat{U}_T$?

2. Consider first class A, which does not impose any symmetries on the Hamiltonian. Prove that by adding a term $m\hat{\mathcal{C}}$, one gets a gapful Hamiltonian $\hat{H}'_{\text{surf}} = \hat{H}_{\text{surf}} + m\hat{\mathcal{C}}$. This statement means that the class A in $3D$ is topologically trivial.
Hint: consider $\hat{H}'^2_{\text{surf}}$.

3. The mass term $m\hat{\mathcal{C}}$ violates both chiral and time-reversal symmetries, thus making classes $AIII$ and AII topologically non-trivial (this term is forbidden in these classes, which possess the chiral and time-reversal symmetries, respectively). In order to distinguish between $\mathbb{Z}$ and $\mathbb{Z}_2$ topological indices, let us now consider two copies of the system, and ask whether one can add a perturbation which mixes two blocks and opens a gap:

$$\hat{H} = \begin{pmatrix} \hat{H}_{\text{surf}} & \hat{V} \\ \hat{V}^\dagger & \hat{H}_{\text{surf}} \end{pmatrix}. \tag{8}$$

Show that there exists a matrix $\hat{V}$, which leads to the gap opening, and which preserves time-reversal symmetry $\hat{\mathcal{T}} = (\hat{U}_T \otimes \hat{\mathbb{I}})\mathcal{K}$ (here $\hat{\mathbb{I}}$ is a unit matrix in the copies space) but breaks chiral symmetry $\hat{\mathcal{C}} \otimes \hat{\mathbb{I}}$. The possibility to open a gap for two copies of the system without symmetry breaking corresponds to the $\mathbb{Z}_2$ classification. When such a mass term breaks the symmetry of the class, one has the $\mathbb{Z}$ classification.
Hint: a gap opens iff the equation $\det \hat{H}(k_1, k_2) = 0$ has no solutions.