Topological Systems: Worksheet 2

Chern insulator and BHZ model

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The minimal model for a two-band Chern insulator is given by the following continuum Hamiltonian:

$$H_0(\boldsymbol{k}) = A(k_x\sigma_x + k_y\sigma_y) + (M - Bk^2)\sigma_z$$

where A, M, and B are real parameters and $k = |\boldsymbol{k}|$ with $\boldsymbol{k} = (k_x, k_y)$. Here, the Pauli matrices correspond to an orbital degree of freedom and not spin. The *Bernevig-Hughes-Zhang* (BHZ) model essentially consists of two copies of a Chern insulator, one for each spin:

$$H_{\text{BHZ}}(\boldsymbol{k}) = \begin{pmatrix} H_0(\boldsymbol{k}) & 0 \\ 0 & H_0(-\boldsymbol{k})^* \end{pmatrix},$$

where $H_0(-\boldsymbol{k})^*$ is the time-reversed version of $H_0(\boldsymbol{k})$.

(1) Show that the BHZ Hamiltonian has time-reversal symmetry:

$$H_{\text{BHZ}}(\boldsymbol{k}) = TH_{\text{BHZ}}(-\boldsymbol{k})T^{-1},$$

where $T = is_yK$ is the time-reversal operator for spin-1/2 fermions, where s_y corresponds to the spin in contrast to σ_y.

(2) Find the energy eigenvalues and normalized eigenstates of the BHZ model. Hint: Treat the two spins independently.

(3) Consider the eigenstates at $k = 0$ and $k \to \infty$. What are the conditions that these eigenstates are different and what parameters have to be tuned to change them?

(4) Write the Hamiltonian for the Chern insulator as

$$H_0(\boldsymbol{k}) = d_x(\boldsymbol{k})\sigma_x + d_y(\boldsymbol{k})\sigma_y + d_z(\boldsymbol{k})\sigma_z = \boldsymbol{d}(\boldsymbol{k}) \cdot \boldsymbol{\sigma},$$

and plot the vector $\hat{\boldsymbol{n}} = \boldsymbol{d}/|\boldsymbol{d}|$ in momentum space. Discuss its topological properties depending on the parameters M and B.

(5) Consider a semi-infinite plane $x \leq 0$. In this case, the momentum in the k_x direction is not a good quantum number. Make the substitution $\boldsymbol{k} \to -i\nabla$ and take the *ansatz*:

$$\Psi_{k_y}(\boldsymbol{r}) = e^{ik_y y}\psi(x), \qquad \psi(x) = e^{\lambda x}\phi_\lambda.$$

Set $k_y = 0$ and find the values of λ that satisfy $H_0(-i\partial_x, k_y = 0)\psi = E\psi$. You should find four different solutions for λ in general:

$$\lambda_\pm^2 = \frac{A^2 - 2BM \pm \sqrt{A^2\left(A^2 - 4BM\right) + 4B^2E^2}}{2B^2}, \quad \phi_\lambda = \begin{pmatrix} M + B\lambda^2 + E \\ -iA\lambda \end{pmatrix}.$$

Hence the general solution for $k_y = 0$ is given by

$$\psi_0(x) = \sum_\lambda c_\lambda e^{\lambda x}\phi_\lambda,$$

where c_λ are unknown coefficients determined by boundary conditions: (a) the wave function should be normalizable in $x \leq 0$ and (b) $\psi(0, y) = 0$. Use these boundary conditions to find an equation for the c_λ. Show that it gives the condition

$$B\lambda_1\lambda_2 = M + E,$$

where $\lambda_{1,2}$ are those of the four λ for which the boundary condition can be satisfied. Solve it for E by squaring it and show that one solution is given by $E = 0$. Prove that for this solution to be consistent with the boundary conditions, we require $M/B > 0$. Now show that the other solution $E = -M$ is inconsistent with the boundary conditions.

(6) Write down the wave function of the zero-energy solution. You should find

$$\phi_0(x) = a \begin{bmatrix} M + B\lambda_1^2 \\ -iA\lambda_1 \end{bmatrix} \left(e^{\lambda_1 x} - e^{\lambda_2 x}\right),$$

where a is a normalization constant.

(7) Find the solutions of exercise (6) for the BHZ model by using the time-reversal symmetry operator T. These two zero-energy solutions form a Kramers pair.

(8) Use the solutions for $k_y = 0$ and use perturbation theory to find the solutions at small k_y:

$$H_{\mathrm{BHZ}} = H_{\mathrm{BHZ}}(k_y = 0) + \left[H_{\mathrm{BHZ}} - H_{\mathrm{BHZ}}(k_y = 0)\right],$$

where the second part is the perturbation in k_y. Show that

$$\begin{bmatrix} \langle\psi_1| V |\psi_1\rangle & \langle\psi_1| V |\psi_2\rangle \\ \langle\psi_2| V |\psi_1\rangle & \langle\psi_2| V |\psi_2\rangle \end{bmatrix} = \hbar v k_y s_z$$

in lowest order of k_y and where $|\psi_{1,2}\rangle$ are the zero-energy Kramers partners with $V = H_{\mathrm{BHZ}} - H_{\mathrm{BHZ}}(k_y = 0)$. Find an expression for v.

(9) Consider again the bulk system and calculate the Berry connection

$$\boldsymbol{A}_s(\boldsymbol{k}) = i \langle u_{s\boldsymbol{k}}| \nabla_{\boldsymbol{k}} |u_{s\boldsymbol{k}}\rangle,$$

where $|u_{n\boldsymbol{k}}\rangle$ are normalized eigenstates of $H_0(\boldsymbol{k})$ with $s = \pm 1$ labeling the two bands. Calculate the line integral around the origin at fixed energy E_F for $B = 0$ and $M/Ak_F \ll 1$.

(10) Calculate the Berry curvature

$$F_{xy}(\boldsymbol{k}) = \partial_{k_x} A_y - \partial_{k_y} A_x,$$

for the lowest-energy band. Make a plot of $F_{xy}(\boldsymbol{k})$ in $\boldsymbol{k}$-space and discuss its form near $\boldsymbol{k} = 0$ when M/B changes sign. Numerically calculate the Chern number of the lowest-energy band:

$$\mathcal{C} = \frac{1}{2\pi} \int_{\mathbb{R}_2} d\boldsymbol{k}\, F_{xy}(\boldsymbol{k}),$$

and show that it is quantized to 0 or ± 1. Make a phase diagram.

(11) Show that the Chern number of $H_0(-\boldsymbol{k})^*$ is opposite to that of $H_0(\boldsymbol{k})$, which is a consequence of time-reversal symmetry, and define the spin Chern number $(\mathcal{C}_\uparrow - \mathcal{C}_\downarrow)/2$.

(12) Why is the Chern number quantized even though the momentum space of our model is not compact ($\boldsymbol{k} \in \mathbb{R}^2$). Hint: consider the case $k \to \infty$ and argue why momentum space is effectively equivalent to a sphere for this model.