

Problem 1. The quantum anomalous Hall effect in a square lattice model

The entire homework this week will be dedicated to solving on specific model, replicating the work we did for the Haldane model. Part of this work will include *model building*. In order to understand what we mean, in the Haldane model we introduced hoppings it_2 which made the gap at Dirac nodes change sign driving us from trivial to topological. In this problem, you will need to discover a term that does the same thing. It is therefore *crucial* that you make sure each part is correct before moving on.

The base model we will consider a tight-binding model with spin on a square lattice (lattice spacing $a = 1$)

$$H_1 = \sum_{\mathbf{r}} (it_1\sigma_x \otimes |\mathbf{r} + \hat{\mathbf{x}}\rangle \langle \mathbf{r}| + it_1\sigma_y \otimes |\mathbf{r} + \hat{\mathbf{y}}\rangle \langle \mathbf{r}| + \text{h.c.}). \quad (1)$$

Throughout, we will consider the chemical potential to be at $E = 0$ (the entire lower band will be filled.)

- (a) Rewrite this Hamiltonian in momentum space. (Do not diagonalize in the spin basis represented by the Pauli matrices σ_x and σ_y .) What are the energy bands $E_{\pm}(\mathbf{k})$ (for the two bands labeled by \pm)?
- (b) *Dirac nodes*: Where does $E_+(\mathbf{k}) = E_-(\mathbf{k}) = 0$? (Hint: there should be 4 points in the Brillouin zone.) Expand the Hamiltonian about each point to obtain Dirac nodes. What are the *helicities* of each Dirac node? [Helicity is defined by $\delta = \text{sgn}(ab)$ for $h = ak_x\sigma_x + bk_y\sigma_y$.]
- (c) Add in a *Zeeman* energy term

$$H_{\Delta} = \Delta \sum_{\mathbf{r}} \sigma_z \otimes |\mathbf{r}\rangle \langle \mathbf{r}|. \quad (2)$$

With this term answer the following: How does this modify the Dirac nodes in (b)? What is the Berry curvature Ω_{k_x, k_y} near each Dirac node? And as a result, what is each Dirac nodes contribution to σ_{xy} ? Lastly, what is the total σ_{xy} ?

- (d) With $H = H_1 + H_{\Delta}$, draw a 3D picture of the Brillouin zone and Δ on the third axis. Indicate where all four Berry monopoles are and their charges (i.e., helicities). How does this explain σ_{xy} from part (c)?
- (e) Staying purely in momentum space, construct an $H_2(\mathbf{k})$ across the entire Brillouin zone that “moves” the monopoles around and can drive a topological phase transition. Some hints: (1) $H_2(\mathbf{k})$ should look like $+t_2\sigma_z$ at one Dirac node and $-t_2\sigma_z$ at the other Dirac nodes (this is not the only way one can do this – consider what we need to change to realize different Chern numbers). (2) Away from those nodes they should be at most quadratic in momentum. (i.e., If the Dirac node is at \mathbf{K}_D and has positive helicity, then $H_2(\mathbf{K}_D + \mathbf{q}) = t_2\sigma_z + O(q^2)$.) (3) To make simpler models in real space use only terms that are σ_z multiplied by 1, $\sin(k_x)$, $\cos(k_x)$, $\sin(k_y)$, or $\cos(k_y)$.

- (f) With the $H_2(\mathbf{k})$ from part (e), rewrite it as a tight-binding model in real space such as how Eqs. (1) and (2) look like.
- (g) Determine where the topological phase transition occurs for your full constructed model $H = H_1 + H_\Delta + H_2$ and draw a phase diagram of t_1/Δ vs. t_2/Δ and indicate the different topological phases.

Problem 2. Numerically solving the model

In this problem, we will use $H = H_1 + H_\Delta + H_2$ from the previous problem only implemented on the full tight-binding model numerically. Much of this is a reworking of the code HALDANE_BSR.PY (part b), HALDANE_BCURV.PY (part c), and HALDANE_TOPO.PY (part d).

Implement the model with PYHTTB.PY. While we have used the language of spin, it might be useful to use orbitals both located at point $\mathbf{r} = (0, 0)$ in the unit cell. For instance, we can implement Eqs. (1) and (2) with

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lattice_vecs = [[1.0, 0.0], [0.0, 1.0]]
orb_positions = [[0.0, 0.0], [0.0, 0.0]]
model = tb_model(2, 2, lattice_vecs, orb_positions)
model.set_onsite([-delta, delta])
model.set_hop(t1 * 1.j, 0, 1, [1, 0])
model.set_hop(t1 * 1.j, 1, 0, [1, 0])
model.set_hop(t1, 1, 0, [0, 1])
model.set_hop(-t1, 1, 0, [0, 1]).
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(This code does not implement H_2 .)

- Write out the code used to implement your H_2 from Problem 1.
- Compute dispersions along the path in the square Brillouin zone $\Gamma = (0, 0)$ to $X = (\pi, 0)$ to $M = (\pi, \pi)$ and back to Γ for 4 cases: $H_2 = 0$, and for $H_2 \neq 0$ but in topological phase, trivial phase, and at the transition points. Mark the band inversion at the high-symmetry point (if your model is not captured by the above path, modify the path to include it). Plot these four cases.
- Compute and plot the Berry curvature (level curves, color plot, or 3d plot) across the whole Brillouin zone for $H_2 = 0$, and for $H_2 \neq 0$ in both trivial and topological phases. (3 plots total.)
- For a ribbon/cylinder geometry plot the hybrid Wannier centers as defined by Berry phase along with the edge band structure in the trivial and topological phases. This shows both *charge pumping* and *edge states* in the model you created!