Sheet 7:

Hand-out: Tuesday, Dec. 05, 2023; Solutions: Tuesday, Dec. 12, 2023

Problem 1 Topological charge of a Dirac cone

Consider the following Hamiltonian describing a Dirac cone:

$$\hat{\mathcal{H}}(\boldsymbol{k}) = \boldsymbol{k} \cdot \boldsymbol{\sigma}, \tag{1}$$

where $\boldsymbol{\sigma}$ is a vector of Pauli matrices. This two-band Hamiltonian is gapped everywhere except at $\boldsymbol{k} = 0$, where the fully linear dispersion realizes a Dirac cone.

(1.a) Consider a loop $\mathcal{C}(k_z)$ in the parameter space, on the surface of a sphere or radius $k_0 > 0$, defined as follows:

$$\mathcal{C}(k_z) = \{\boldsymbol{k} | \boldsymbol{k} \cdot \boldsymbol{e}_z = k_z, \boldsymbol{k}^2 = k_0\}. \tag{2}$$

Show that the corresponding Berry phase vanishes when $k_z = \pm k_0$:

$$\varphi_{\mathrm{B}}(k_z = \pm k_0) \equiv 0 \mod 2\pi. \tag{3}$$

(1.b) For $-k_0 < k_z < k_0$, calculate the Berry phase φ_{B} corresponding to $\mathcal{C}(k_z)$. *Hint:* Write the eigenfunctions of $\hat{\mathcal{H}}(\boldsymbol{k})$ as a function of $\boldsymbol{k}$ in cylindrical coordinates $\boldsymbol{k} = (k_r \cos(\phi), k_r \sin(\phi), k_z)$ with $k_r^2 + k_z^2 = k_0^2$.

(1.c) The family of curves $\mathcal{M} = \{\mathcal{C}(k_z) | k_z = -k_0 ... k_0\}$ define a manifold in parameter-space: A sphere of radius k_0 around the Dirac cone. Using your result in (2.b), show by an explicit calculation that the topological invariant $C_{\mathcal{M}}$ associated with $\mathcal{M}$ is

$$C_{\mathcal{M}} = 1. \tag{4}$$

I.e. the Dirac cone is associated with a unit topological charge $C_{\mathcal{M}} = 1$.

(1.d) In (2.b) you will find in the equatorial plane that:

$$\varphi_B(k_z = 0) \equiv \pm\pi \mod 2\pi. \tag{5}$$

Derive this result from symmetry considerations alone. Show that from inversion $\boldsymbol{k} \to -\boldsymbol{k}$ it follows that

$$\varphi_{\mathrm{B}}(-k_z) \equiv -\varphi_{\mathrm{B}}(k_z) \mod 2\pi, \tag{6}$$

and combine this with $C_{\mathcal{M}} = 1$ from (2.c).

Problem 2 Edge states in the non-interacting SSH model

Consider the non-interacting SSH dimer chain described by the Hamiltonian (L even):

$$\hat{H} = -t_1 \sum_{j=1}^{L/2} \left(\hat{a}_j^\dagger \hat{b}_j + \text{h.c.} \right) - t_2 \sum_{j=1}^{L/2-1} \left(\hat{a}_{j+1}^\dagger \hat{b}_j + \text{h.c.} \right), \tag{7}$$

with open boundary conditions.

Remark: This problem closely follows [Delplace et al., PRB 84, 195452 (2011)].

(2.a) For periodic boundary conditions, the bulk wavefunctions are Bloch waves. Introduce

$$\hat{\Psi}_k = \left(\hat{\psi}_{A,k}, \hat{\psi}_{B,k} \right)^T = (L/2)^{-1/2} \sum_{j=1}^{L/2} e^{-ijk} \left(\hat{a}_j, \hat{b}_j \right)^T \tag{8}$$

and show that that

$$\hat{H} = \sum_{k_n = n2\pi/M} \hat{\Psi}_k^\dagger \hat{\mathcal{H}}(k_n) \hat{\Psi}_k, \qquad n = 1, ..., L/2, \tag{9}$$

where the Bloch Hamiltonian is

$$\hat{\mathcal{H}}(k) = t_2 \, \boldsymbol{g}(k) \cdot \hat{\boldsymbol{\sigma}}, \qquad \boldsymbol{g}(k) = (\mathrm{Re}\rho(k), \mathrm{Im}\rho(k))^T, \tag{10}$$

where $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}^x, \hat{\sigma}^y)$ and $\rho(k) = t_1/t_2 + e^{-ik}$.

(2.b) You may write $\boldsymbol{g}(k)$ from (3.a) as:

$$\boldsymbol{g}(k) = |\rho(k)| \left(\cos\phi(k), \sin\phi(k) \right)^T, \qquad \cot\phi(k) = \frac{t_1}{t_2 \sin k} + \cot k. \tag{11}$$

Use this result to show that the cell-periodic Bloch functions are

$$|u_k^\pm\rangle = \frac{1}{\sqrt{2}} \left(e^{-i\phi(k)}, \pm 1 \right)^T. \tag{12}$$

Further, show that the corresponding Zak phase is $\varphi_{\text{Zak}} = 0$ ($\varphi_{\text{Zak}} = \pi$) for $t_1 > t_2$ ($t_1 < t_2$). Sketch the line parameterized by $\boldsymbol{g}(k)$ in the two-dimensional plane and show that its topology changes at $t_1 = t_2$ – note that $\boldsymbol{g}(k) = 0$ is special because it corresponds to a closing of the band gap.

(2.c) Now we consider *open* boundary conditions. The bulk wavefunctions $|v_k^\mu\rangle$ are standing waves ($k \geq 0$) and can be constructed as superpositions of $|u_k^\mu\rangle$ and $|u_{-k}^\mu\rangle$, with $\mu = \pm$ the band index. Explain why the following boundary conditions must be satisfied,

$$\langle j = 0, B | v_k^\mu \rangle = 0, \qquad \langle j = L/2 + 1, A | v_k^\mu \rangle = 0, \tag{13}$$

where $|j, \alpha\rangle$ denotes site $\alpha = A, B$ in the unit-cell at position $j = 1...L/2$.

(2.d) Using $\phi(-k) = -\phi(k)$, show that the bulk eigenfunctions $|v_k^\mu\rangle$ may be written as

$$|v_k^\mu\rangle = \frac{i}{\sqrt{L/2}} \sum_{j=1}^{L/2} \big[\sin\left(kj - \phi(k)\right)|j, A\rangle + \mu \sin\left(kj\right)|j, B\rangle\big], \tag{14}$$

and derive the quantization condition for $0 < k < \pi$:

$$k\left(\frac{L}{2} + 1\right) - \phi(k) = n\pi, \qquad n \in \mathbb{Z}. \tag{15}$$

(2.e) Sketch the functions $\phi(k)$ and $k(L/2+1) - n\pi$ – their intersections correspond to solutions of the quantization condition in (3.d). Use the different topology of $\boldsymbol{g}(k)$ [and, correspondingly, of $\phi(k)$] to show that the number of solutions depends on the ratio of t_1/t_2. Specifically, show that $L/2$ solutions exist when $t_1 > \lambda_c t_2$ and $L/2 - 1$ solutions exist when $t_1 < \lambda_c t_2$, where

$$\lambda_c = \left(\frac{t_1}{t_2}\right)_c = 1 - \frac{1}{L/2+1} \to 1 \qquad \text{for} \;\; L \to \infty. \tag{16}$$

I.e. a bulk state is missing in the case when the Zak phase is $\phi_{\mathrm{Zak}} = \pi$.

(2.f) For $t_1 < \lambda_c t_2$ [i.e. when the Zak phase is $\phi_{\mathrm{Zak}} = \pi$] one can similarly construct edge states. This is achieved by looking for solutions as in Eq. (14) but with a wavevector: $k = \pi + i\kappa$, where $1/\kappa = \xi$ is the localization length at the edge. The solution (no derivation is necessary!) is given by:

$$|e_\kappa^\mu\rangle = \frac{1}{\sqrt{L/2}} \sum_{j=1}^{L/2} (-1)^{j+1} \big[a_{\kappa,j}^\mu |j, A\rangle + b_{\kappa,j}^\mu |j, B\rangle\big], \tag{17}$$

with eigenenergies $\varepsilon_\kappa^\mu = \mu t_2 |\rho(i\kappa)|$ where:

$$\begin{pmatrix} a_{\kappa,j}^\mu \\ b_{\kappa,j}^\mu \end{pmatrix} = \begin{pmatrix} \sinh\big(\kappa(L/2 + 1 - j)\big) \\ \mu \sinh\left(\kappa j\right) \end{pmatrix} \tag{18}$$

and κ satisfies the following quantization condition:

$$t_1 \sinh\big(\kappa(L/2+1)\big) = t_2 \sinh\left(\kappa L/2\right). \tag{19}$$

Use these results to show for large $L \gg 1$ that

$$t_1/t_2 \simeq \exp\left(-\kappa\right), \tag{20}$$

which leads to:

$$\varepsilon_\kappa^\mu \simeq \mu \exp\left(-\kappa L/2\right). \tag{21}$$

Discuss the physical meaning of these results!