Field Theory in Condensed Matter (2023-2024)

Exercise Series on Quantum Geometry and Topology – 2

1 Quantization of polarization and topology in 1D – The SSH model (HOMEWORK)

In this exercise we consider a 1D tight-binding model of the Hamiltonian for an electron hopping on a chain subject to a periodic dimerization. This model was first devised by Su, Shrieffer and Heeger to model solitons on a polyacetylene polymer chain [PRL **42**, 1698 (1979)]. The Hamiltonian is given by

$$\mathcal{H} = t_1 \sum_{i=j}^{N} c_{2j-1}^{\dagger} c_{2j} + t_2 \sum_{i=1}^{N} c_{2j}^{\dagger} c_{2j+1} + \text{h.c.} \tag{1}$$

where t_1 and t_2 are hopping amplitudes and $c_j^{\dagger}$ (c_j) is the creation (annihilation) operator for an electron at site $x_j = ja$ of the chain, where a is the lattice spacing. Periodic boundary conditions are implied and h.c. stands for *hermitian conjugate*. The operators obey the canonical anticommutation relations for fermionic operators,

$$\{c_i^{\dagger}, c_j\} = \delta_{ij}$$
$$\{c_i, c_j\} = 0.$$

a) One can split the chain into two sublattices A and B. Find a suitable definition of canonical sublattice operators such that you can write

$$\mathcal{H} = t_1 \sum_{i=1}^{N} c_{i,A}^{\dagger} c_{i,B} + t_2 \sum_{i=1}^{N} c_{i,B}^{\dagger} c_{i+1,A} + \text{h.c.}$$

b) Diagonalize this Hamiltonian by using the momentum space operators

$$c_{,k_m} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{\mathrm{i} k_m x_j} c_{\sigma,j}$$

where $k_m = 2\pi m/Na$. Show that in this basis, after taking the $N \to \infty$ limit, the Hamiltonian can be written as

$$\mathcal{H} = \int_0^{2\pi/a} \frac{\mathrm{d}k}{2\pi} \mathbf{C}^{\dagger}(k) H(k) \mathbf{C}(k)$$

with the Bloch Hamiltonian

$$H(k) = \mathbf{d}(k) \cdot \boldsymbol{\tau},$$

where $\mathbf{C}(k) \equiv (c_A(k), c_B(k))^T$ and $\boldsymbol{\tau} \equiv (\sigma_x, \sigma_y, \sigma_z)^T$ is a vector of Pauli matrices. Write down the vector $\mathbf{d}(k)$ explicitely and show that the dispersion relation is given by

$$E_{\pm}(k) = \pm\sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos ka} \tag{2}$$

c) Show that the eigenstates of a **generic** 2×2 Bloch Hamiltonian $H(k) = \mathbf{d}(k) \cdot \boldsymbol{\tau}$ can be written as

$$|\psi_{\pm}(k)\rangle = \frac{1}{\sqrt{2(d(k)(d(k) \pm d_3(k)))}} \begin{pmatrix} d_3(k) \pm d(k) \\ d_1(k) + \mathrm{i}d_2(k) \end{pmatrix},$$

up to a gauge transformation.

d) Consider the chiral (sublattice) transformation:

$$\Gamma : \begin{pmatrix} c_{i,A} \\ c_{i,B} \end{pmatrix} \to \begin{pmatrix} c_{i,A} \\ -c_{i,B} \end{pmatrix}.$$

Show that in order for the Hamiltonian $\mathcal{H}$ to be symmetric under Γ, the Bloch Hamiltonian has to transform as

$$H(k) \to -H(k).$$

Find the matrix representation of this transformation on the Bloch Hamiltonian. What are the consequences of this symmetry on the single-particle spectrum and eigenstates?

e) Show that the Hamiltonian also has an inversion symmetry across the center of the unit cell. Find the matrix representation that performs this transformation. The Bloch Hamiltonian should transform as

$$H(k) \to H(-k)$$

The combination of these two symmetries has interesting consequences on the polarization properties of this system. Inversion symmetry forces the quantization of polarization to two values, a result that holds for all inversion-symmetric 1D systems, as was shown by Zak [PRL **62**, 2747 (1989)]. On the other hand, sublattice symmetry allows for an interpretation of this quantization in terms of a topological invariant, providing us with one of the simplest example of a *bulk-boundary correspondence* for topological insulators. We will now explore this connection. We will furthermore also set $a = 1$ for simplicity.

f) Sublattice symmetry enforces that the vector component $d_3(k) = 0$. Recall that the winding number of a function $\mathbf{d} : S^1 \to \mathbb{R}^2$ is defined by

$$\nu = \oint_C \frac{\mathrm{d}\phi}{2\pi},$$

where $\phi(k)$ is the polar angle of the 2D vector $\mathbf{d}(k)$, given by

$$\phi = \arctan\left(\frac{d_y(k)}{d_x(k)}\right),$$

and C is a closed contour on the (d_1, d_2) plane. Show that the winding number takes the values $0, 1$ according to the following condition

$$\nu = \begin{cases} 0, & \text{if } |t_1| > |t_2| \\ 1, & \text{if } |t_1| < |t_2| \end{cases} \tag{3}$$

g) Consider the SSH chain at half-filling. That is, the lower band of this system is completely filled and we have an insulator. The polarization density is given by

$$P = \frac{\gamma}{2\pi}$$

(modulo a quanta of charge), where γ is the Berry phase of the system. By explicitly calculating the Berry phase, show that

$$P = \frac{1}{2}\nu,$$

where ν is the winding number given by Eq. (3). From Eq. (2), we see that the system has to undergo a topological phase transition at $t_1 = t_2$ by closing the insulating gap in order to attain the trivial phase, with $t_1 > t_2$.

If the system is cut open while respecting inversion symmetry of the unit cells, the ground state of this system, when $t_1 < t_2$ will be composed of a filled Fermi sea and an additional electron occupying two degenerate zero-energy edge modes. This is why the physical picture of polarization consists of half charges sitting at the two ends of the system whenever it is in the "topological" phase.
Let us now explicitly show the bulk-boundary correspondence by determining the condition for the existence of zero-energy edge modes. In order to do this, we will employ a transfer matrix approach.

h) Consider the first quantized Hamiltonian from (1) for a single electron,

$$H = t_1 \sum_{j=1}^{N} |j, A\rangle \langle j, B| + t_2 \sum_{j=1}^{N} |j, B\rangle \langle j+1, A| + \text{h.c}$$

where $|j, A\rangle$ is a basis state for a single electron in the unit cell j, on sublattice A. Let

$$|\psi\rangle = \sum_{j=1}^{N} a_j |j, A\rangle + b_j |j, B\rangle$$

be a zero-energy eigenstate. Show that the two possible solutions to the matrix equation are given by

$$a_j = a\left(-\frac{t_1}{t_2}\right)^{j-1}, \quad \text{for } 1 \leq j \leq N-1,$$
$$b_j = b\left(-\frac{t_1}{t_2}\right)^{-j+N}, \quad \text{for } 2 \leq j \leq N.$$

where a and b are arbitrary constants. Under which condition are these states physical? These states are localized on the edges of the system. Determine their localization length.

We have now fully established the bulk-boundary correspondence in the SSH chain.