

EXERCISE: Two-dimensional Chiral Superconductors

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1 Chern number due to a winding function

The Chern number, an integer Ch , is a famous topological invariant that can characterize gapped Hamiltonians of two-dimensional (2d) systems. In some particular cases, the Hamiltonian can be expressed using different mathematical objects, each with its type of topological integer, all of which have the same value. In this problem, we will study an example of such a situation, where the topology of a given 2x2 Hamiltonian of a superconductor in 2d (in class D) is given by Ch . The Ch takes the form of an integer wrapping number of a 2d surface around the origin, which can be calculated algebraically. The second goal is to show that the Ch also equals the winding number W of an angle (the phase of the pairing function) around a closed curve (the Fermi surface).

1.1 Finding the Hamiltonian matrix

(a) Consider the following second quantized Hamiltonian in two dimensions:

$$\hat{H} = \sum_{\mathbf{k} \in \text{BZ}} (\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k} \in \text{BZ}} \left(\Delta_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{-\mathbf{k}}^{\dagger} + \Delta_{\mathbf{k}}^* c_{-\mathbf{k}} c_{\mathbf{k}} \right), \quad (1)$$

where $c_{\mathbf{k}}$ annihilates an electron at momentum $\mathbf{k} = (k_x, k_y)$, and we assume for simplicity that the kinetic energy $\varepsilon_{\mathbf{k}}$ is an even function of $\mathbf{k}$.

Find the 2x2 Hamiltonian matrix $H_{\mathbf{k}}$ of $\hat{H}$, using the definition

$$\hat{H} = \frac{1}{2} \sum_{\mathbf{k} \in \text{BZ}} \psi^{\dagger} H_{\mathbf{k}} \psi + \text{const}, \quad \psi \equiv \begin{pmatrix} c_{\mathbf{k}} \\ c_{-\mathbf{k}}^{\dagger} \end{pmatrix}. \quad (2)$$

HINT 1: Your final result should be $H_{\mathbf{k}} = \begin{pmatrix} \varepsilon_{\mathbf{k}} - \mu & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & -(\varepsilon_{-\mathbf{k}} - \mu) \end{pmatrix}$.

HINT 2: To find the bottom-right matrix element, you can rewrite the kinetic energy by changing $\mathbf{k} \rightarrow -\mathbf{k}$ in the sum, and use $\{c_{\mathbf{k}}, c_{\mathbf{k}}^{\dagger}\} = 1$.

The second quantized Hamiltonian $\hat{H}$ is a description of a superconductor. The function $\Delta_{\mathbf{k}}$ is called the “pairing function” as it describes the quantum amplitude of creating a Cooper pair of electrons ($c^{\dagger} c^{\dagger}$).

1.2 Band structure

1.2.1 Without pairing

(b) We will first consider the system without pairing $\Delta_{\mathbf{k}} \equiv 0$. The correct band structure of this unpaired system is just $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$. We now model the kinetic energy $\varepsilon_{\mathbf{k}}$. Consider the nearest-neighbor tight-binding model on a square lattice (Fig. 1a): $H^{\text{square}} =$

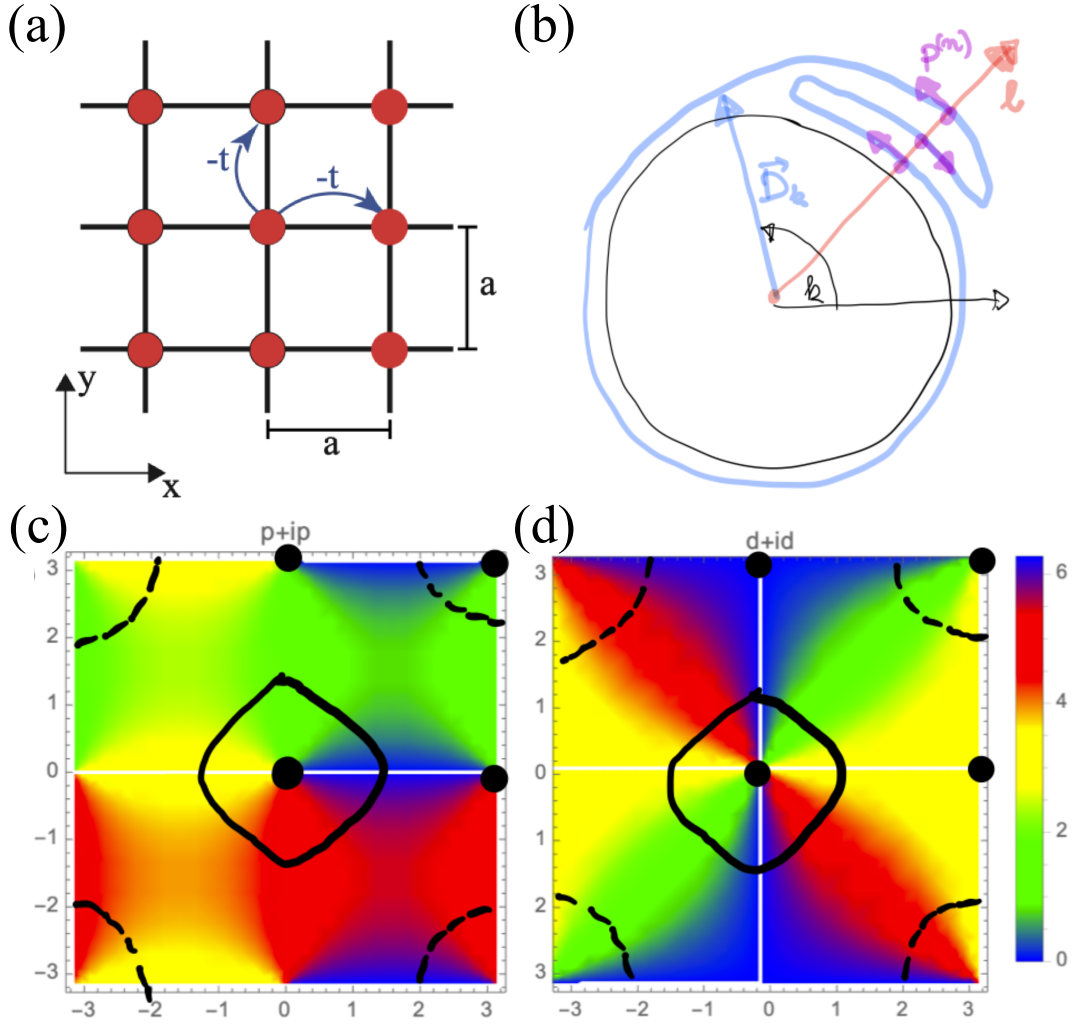


Figure 1: (a) Nearest-neighbor tight-binding model on square lattice, each site $\vec{R}_i \equiv (x_i, y_i)$ carries one state $|i\rangle$. (b) Illustration of the algebraic method to calculate how many times a hyper-surface (here, a planar curve in two dimensions, blue line) wraps around the origin (black dot). One only needs to find intersection points (purple dots) with a ray (red line) and properly count their orientations (here, direction of purple tangential vectors). (c) Phase $\varphi_{\mathbf{k}}$ of the pairing function $\Delta_{\mathbf{k}}^{1+}$ (“ $p+ip$ ”) throughout the Brillouin Zone (BZ). The Fermi surface (FS) of the unpaired state, defined by $\xi_{\mathbf{k}} \equiv 0$ is given for examples of $\mu \gtrsim -2t$ (full line) vs. $\mu \lesssim 2t$ (dashed line). (d) Same as (c), but for $\Delta_{\mathbf{k}}^{2+}$ (“ $d+id$ ”).

$\sum_{\langle i,j \rangle} (-t |i\rangle \langle j| + h.c.)$, where each nearest-neighbor unordered pair of sites $\langle i,j \rangle$ on the lattice is counted once, and $t > 0$ is a real positive constant. You may assume periodic boundary conditions with the same N number of lattice sites in both x and y direction, and set the lattice constant as unit of length, $a \equiv 1$. Show that the energy dispersion of H^{square} is $\varepsilon_{\mathbf{k}}^{square} = -t(\cos(k_x) + \cos(k_y))$. Show that the first Brillouin Zone (BZ) is $k_x \in (-\pi, \pi]$, $k_y \in (-\pi, \pi]$.

From now on, we will set the kinetic energy as $\varepsilon_{\mathbf{k}} \equiv \varepsilon_{\mathbf{k}}^{square}$. **The Fermi Surface (FS) of the unpaired system is defined by the $\mathbf{k}$ that satisfy $\xi_{\mathbf{k}} \equiv 0$.** The FS of the unpaired system is either absent (if $|\mu| > 2t$) or it forms a contour in the BZ (see Fig. 1c,d).

1.2.2 With pairing

- (c) When $\Delta \neq 0$, the correct Hamiltonian matrix is the 2x2 $H_{\mathbf{k}}$, which can be written using a three-component vector $H_{\mathbf{k}} = \vec{D}_{\mathbf{k}} \cdot \vec{\sigma}$ with the usual Pauli matrices¹.

Find the $\vec{D}_{\mathbf{k}}$, and express the band structure $E_{\mathbf{k}}$ of $H_{\mathbf{k}}$ in terms of $\xi_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}$.

- (d) We now introduce four separate models by also fixing the pairing function $\Delta_{\mathbf{k}}$ as one of four different possibilities²:

$$\Delta_{\mathbf{k}}^{1\pm} = \Delta_0 [\sin(k_x) \pm i \sin(k_y)] \quad (3)$$

$$\Delta_{\mathbf{k}}^{2\pm} = \Delta_0 [\cos(k_x) - \cos(k_y) \pm i \sin(k_x) \sin(k_y)], \quad (4)$$

which are called " $p \pm ip$ " and " $d \pm id$ ", respectively. We shall call $H_{\mathbf{k}}^{P\pm}$ the model in which $\Delta_{\mathbf{k}} \equiv \Delta_{\mathbf{k}}^{P\pm}$, with $P = 1, 2$.

In the following we consider μ as the only variable parameter ($t, \Delta_0 > 0$ are fixed) that defines a phase diagram. Find the gapped phases for all four models $H_{\mathbf{k}}^{P\pm}$, $P = 1, 2$.

HINT: Note that the two bands in presence of pairing are $\pm E$ (why?). Hence the bulkgap-closing points appear at values of μ and $\mathbf{k}$ for which the energy $E = 0$.

HINT: You should find that the models $H^{1\pm}$ have four gapped phases (gap closings at $\mu = -2t, 0, 2t$), while the models $H^{2\pm}$ have three gapped phases (gap closings at $\mu = -2t, 2t$).

1.3 Winding of pairing function becomes Chern number

The Hamiltonian $H_{\mathbf{k}}^{P\pm}$, $P = 1, 2$ is spinless and lacks time-reversal symmetry. Being in two dimensions, when it is in a gapped phase it is characterized by the Chern number Ch . This Chern number for our special case of a 2x2 Hamiltonian matrix has a geometrical interpretation: As the momentum $\mathbf{k} = (k_x, k_y)$ covers the entire BZ, the endpoint of the 3-dimensional vector $\vec{D}_{\mathbf{k}} = (D_x(\mathbf{k}), D_y(\mathbf{k}), D_z(\mathbf{k}))$ sweeps out a closed surface, so that Ch equals the number of times this surface wraps around the origin $(0, 0, 0)$. You will calculate Ch geometrically (without integrals) for each gapped phase of all four models $H_{\mathbf{k}}^{P\pm}$. The explanation of the geometric formula for Ch is in a footnote.³

¹We use the standard Pauli matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

²A reinterpretation of $H_{\mathbf{k}}$ occurs at this moment. The derivation of the BdG matrix $H_{\mathbf{k}}$ in the previous section started from effectively spinless single band ($c_{\mathbf{k}}^\dagger$), and in such a case, due to anticommutation $\{c_{\mathbf{k}}^\dagger, c_{-\mathbf{k}}^\dagger\} = 0$ the pairing function $\Delta_{\mathbf{k}}$ can only be odd in $\mathbf{k}$ (or it vanishes), consistent with the " $p \pm ip$ ". However, the exact same form of the BdG matrix $H_{\mathbf{k}}$ is obtained starting from a spinfull problem with spin-singlet pairing, i.e., when the spinor $\psi_{\mathbf{k}} \equiv (c_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}^\dagger)^T$, and the pairing function then is purely even in $\mathbf{k}$ (as in the " $d \pm id$ "). So starting from this point in the exercise, we are using the same form of 2x2 matrix $H_{\mathbf{k}}$ with either an even or odd pairing function, but we should be aware that these describe two different many-body Hamiltonians $\hat{H}$. The careful reader may notice that in the spinfull case the $H_{\mathbf{k}}$ should actually be a 4x4 matrix, since we have two spin orientations ($\uparrow, \downarrow$) and we also have electrons and holes for them. Indeed, but due to the fact that $\hat{H}$ preserves the spin along z -axis (there is no spin-orbit coupling nor triplet pairing), its 4x4 $H_{\mathbf{k}}$ reduces to two separate 2x2 blocks. Actually, the Chern number you calculate for your 2x2 $H_{\mathbf{k}}$ will be the same as the Chern number obtained from the other 2x2 block, so in case of the " $d \pm id$ " the total Chern number of the system is double the one you find.

³We determine the wrapping of $\vec{D}_{\mathbf{k}}$ around the origin by counting how many times the surface $\vec{D}_{\mathbf{k}}$, $\mathbf{k} \in \text{BZ}$ intersects the radial line going from the origin out to infinity along the x -axis, $\vec{l}(a) \equiv (a, 0, 0)$, $a \in [0, +\infty)$. Each time there is an intersection, i.e., there is a solution $(a^{(n)}, \mathbf{k}_x^{(n)}, \mathbf{k}_y^{(n)})$, labeled by n , of the equation $\vec{D}_{\mathbf{k}} \equiv \vec{l}(a)$, we have a contribution to the wrapping number Ch , but each intersection contributes $p^{(n)} = +1(-1)$ if the line intersects the surface from its inside (outside) so as to guarantee that we do not overcount local folds in the surface as wrappings around the origin. The value of $p^{(n)} = \pm 1$ depends simply on whether the local

- (e) Let us consider one gapped phase of one model. The geometrical formula for its Chern number is $Ch = \sum_n p^{(n)}$, where one defines $p^{(n)} \equiv \text{sgn} \left[\vec{D}_{\mathbf{k}} \cdot \left(\partial_{k_x} \vec{D}_{\mathbf{k}} \times \partial_{k_y} \vec{D}_{\mathbf{k}} \right) \right] \Big|_{\mathbf{k}=\mathbf{k}^{(n)}}$, and the values of momenta $\mathbf{k}^{(n)}$, indexed by n , are all the solutions to the “intersection equation” $\vec{D}_{\mathbf{k}} \equiv \vec{l}(a)$, where one defines the ray $\vec{l}(a) \equiv (a, 0, 0)$ with $a \in [0, +\infty)$, while $\mathbf{k}$ is in the first BZ (see Fig. 1c). Find the Ch for each gapped phase of both models $H_{\mathbf{k}}^{\pm}$.

HINT 1: Treat the two models $H_{\mathbf{k}}^{P\pm}$ together using the $\pm$. Find the expression for $p^{(n)}$ for an arbitrary value of μ , and an unknown value $\mathbf{k} \equiv \mathbf{k}^{(n)}$, but profiting from the fact that you know that $\vec{D}_{\mathbf{k}^{(n)}}$ has only an x -component (as does $\vec{l}(a)$). You will plug into this expression the various values of $\mathbf{k}^{(n)}$ you find in different gapped phases determined by the value of μ .
HINT 2: The hard work is in finding all solutions $\mathbf{k} = \mathbf{k}^{(n)}$ of the three simultaneous equations $\vec{D}_{\mathbf{k}} \equiv \vec{l}(a)$. Solve them graphically in the BZ. The key information you need is where the Fermi surface of the unpaired state is, i.e., where is the contour of $\mathbf{k}$ defined by $\xi_{\mathbf{k}} \equiv 0$, and it depends on μ . The key realization is that for $-2t < \mu < 0$ the Fermi surface is a pocket around the Γ point, while for $0 < \mu < 2t$ it is a pocket around the M point (see Fig. 1b).

- (f) Consider the complex phase, $\varphi_{\mathbf{k}}$, of the pairing function, $\exp(i\varphi_{\mathbf{k}}) = \frac{\Delta_{\mathbf{k}}}{|\Delta_{\mathbf{k}}|}$ (see Fig. 1b). Its winding on the unpaired Fermi surface (FS) is

$$W = \frac{1}{L_{FS}} \oint_{FS} d\vec{k} \cdot \nabla_{\vec{k}} \varphi(\vec{k}), \quad (5)$$

with L_{FS} the length of the FS contour. We can pick any value of μ inside a given gapped phase to calculate the W of that gapped phase, since W is topological. However, for any value of μ the integral is hard to solve. We can again use the topological nature of W to deform the FS slightly, as long we don't leave the gapped phase, which is ensured if FS remains to be nearest to the high-symmetry point where it was. Hence, we can deform the FS pocket into a circle. With FS a circle, we have $W = \frac{1}{2\pi} \int_0^{2\pi} d\theta \partial_{\theta} \varphi(\mathbf{k}(\theta))$, where θ is the polar angle around the high-symmetry point $\mathbf{K}$ on which the FS is centered, i.e., $\mathbf{k} \equiv \mathbf{K} + k_F(\cos \theta, \sin \theta)$.

Calculate W for each gapped phase of each of the four models $H_{\mathbf{k}}^{P\pm}$, and confirm that $Ch = W$ if the FS contour is always taken counter-clockwise with respect to the Γ -point.

HINT: The final trick allowed by topology is to consider an infinitesimal FS, i.e., let $k_F \ll 1$ and expand the $\varphi(\mathbf{k}(\theta))$ to linear order.

normal to the surface is parallel (antiparallel) to the line $\vec{l}(a^{(n)})$. Since we have $\vec{l}(a^{(n)}) = \vec{D}(\mathbf{k}^{(n)})$, the $p^{(n)} = \text{sgn} \left[\vec{D}_{\mathbf{k}} \cdot \left(\partial_{k_x} \vec{D}_{\mathbf{k}} \times \partial_{k_y} \vec{D}_{\mathbf{k}} \right) \right]$ is evaluated at $\mathbf{k} = \mathbf{k}^{(n)}$.