Problem set 2 for "Topology in condensed matter"

To be discussed in exercise class on November 21, 2023

1 Semiclassical description of quantum spin

The path integral for quantum spin S involves integration over trajectories of classical vectors of length S. The kinetic term in the corresponding action is precisely given by the Berry phase; if one adopts spherical coordinates $\boldsymbol{S}(t) = S \times (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$, it reads:

$$A_{\text{kin}}[\varphi, \theta] = S \int d\varphi(1 - \cos\theta). \tag{1}$$

If e.g. spin is subject to a constant magnetic field $\boldsymbol{h}$ and is described by the Hamiltonian $\hat{H} = \boldsymbol{h}\hat{\boldsymbol{S}}$, then the total classical action for such problem reads:

$$A[\varphi, \theta] = A_{\text{kin}}[\varphi, \theta] - \int dt\, \boldsymbol{h} \cdot \boldsymbol{S}(t). \tag{2}$$

Show that equations of motion corresponding to this action reproduce the spin precession along the magnetic field:

$$\frac{d\boldsymbol{S}(t)}{dt} = [\boldsymbol{h} \times \boldsymbol{S}(t)]\,. \tag{3}$$

2 Jackiw-Rebbi model

In this exercise you will analyze the two-dimensional *Dirac Hamiltonian*:

$$\hat{H} = v_F(\hat{\sigma}_x k_x + \hat{\sigma}_y k_y) + \Delta\hat{\sigma}_z, \tag{4}$$

with $\hat{\sigma}_\alpha$ being Pauli matrices, and k_α denoting momentum of the particle, assuming $v_F > 0$ and arbitrary sign of Δ.

1. Diagonalize given Hamiltonian, and show that it describes two bands with "relativistic" dispersion $E_\pm(\boldsymbol{k}) = \pm\sqrt{v_F^2\boldsymbol{k}^2 + \Delta^2}$. Find explicitly normalized eigenvectors $|\boldsymbol{k}, \pm\rangle$ corresponding to states with momentum $\boldsymbol{k}$ in these two bands.

2. Calculate the *Chern numbers* of both bands ($n = \pm$):

$$C_n = \frac{1}{2\pi}\int d^2\boldsymbol{k}\, \Omega_n(\boldsymbol{k}), \quad \Omega_n(\boldsymbol{k}) = i\sum_{n' \neq n}\left(\frac{\langle\psi_n|\, \partial\hat{H}(\boldsymbol{k})/\partial k_x\, |\psi_{n'}\rangle \langle\psi_{n'}|\, \partial\hat{H}(\boldsymbol{k})/\partial k_y\, |\psi_n\rangle}{(E_n(\boldsymbol{k}) - E_{n'}(\boldsymbol{k}))^2} - c.c.\right). \tag{5}$$

   Note that obtained Chern numbers are half-integer, which is in apparent contradiction with the statement that Chern numbers for arbitrary band is an integer number. Below we will demonstrate how this contradiction is resolved.

3. Models of this type often arise as the effective low-energy description of some underlying well-defined lattice model (e.g. the gapless model with $\Delta = 0$ describes the low-energy physics of *graphene*). Consider now lattice version of the Dirac Hamiltonian defined on a two-dimensional square lattice (with lattice spacing a), which can be obtained by replacing the momentum operators $\hat{k}_\alpha = -i\nabla_\alpha$ by its finite-difference counterpart:

$$\hat{H}'_{\boldsymbol{r},\boldsymbol{r}'} = (-i)v_F\left(\hat{\sigma}_x\frac{\delta_{x+a,x'}\delta_{y,y'} - \delta_{x-a,x'}\delta_{y,y'}}{2a} + \hat{\sigma}_y\frac{\delta_{x,x'}\delta_{y+a,y'} - \delta_{x,x'}\delta_{y-a,y'}}{2a}\right) + \Delta\hat{\sigma}_z\delta_{x,x'}\delta_{y,y'}. \tag{6}$$

This Hamiltonian is written in the coordinate basis $\boldsymbol{r} = (x, y)$ and $\boldsymbol{r}' = (x', y')$, with coordinates defined on a square lattice $x/a \in \mathbb{Z}$, $y/a \in \mathbb{Z}$. What form does this Hamiltonian acquire in the momentum representation? Check that at small momenta $k_{x,y} \ll a^{-1}$ it reproduces the original Dirac Hamiltonian.

4. Demonstrate that in addition to the center of the Brillouin zone, $\boldsymbol{K}_0 = (0, 0)$, it also contains another set of low-energy states near points $\boldsymbol{K}_1 = (0, \pi/a)$, $\boldsymbol{K}_2 = (\pi/a, 0)$ and $\boldsymbol{K}_3 = (\pi/a, \pi/a)$. Expand the Hamiltonian in the momentum representation near each of these points, $\boldsymbol{k} = \boldsymbol{K}_i + \boldsymbol{p}$, assuming $p \ll a^{-1}$ and show that corresponding expansions $\hat{H}_{1,2,3}(\boldsymbol{p})$ have the form similar to the original Dirac Hamiltonian, albeit with different signs in front of $\hat{\sigma}_x p_x$ and $\hat{\sigma}_y p_y$ terms. It is an illustration of so-called *fermion doubling theorem*: any lattice version of the Dirac Hamiltonian will in general contain an even number of Dirac cones.

5. How does such modification affects the calculation of the Chern numbers performed earlier? In the limit $\Delta \ll v_F/a$, the main contribution to the Chern number comes from the vicinity of points $\boldsymbol{K}_i$ where the Berry curvature is parametrically large. Within this approximation, the integral over the whole Brillouin zone can be calculated as a sum of contributions from the vicinity of each of the points $\boldsymbol{K}_i$. Since each contribution is half-integer, the fermion doubling theorem then guarantees that the total Chern number is integer and provides a resolution to the apparent contradiction observed earlier. What is its value for each of two bands?

6. Now go back to the original Dirac Hamiltonian and consider its spatially inhomogeneous version, which realizes a *boundary* between two topologically distinct bulk phases $\Delta > 0$ and $\Delta < 0$:

$$\hat{H} = v_F(\hat{\sigma}_x \hat{k}_x + \hat{\sigma}_y \hat{k}_y) + \Delta(x)\hat{\sigma}_z, \quad \Delta(x) = \begin{cases} +\Delta_0 & x > 0 \\ -\Delta_0, & x < 0 \end{cases}, \tag{7}$$

assuming $\Delta_0 > 0$, with $\hat{k}_\alpha = -i\partial_\alpha$. Show that it contains special solutions of the following form:

$$|\psi(x)\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \exp\left(-\frac{1}{v_F}\int_0^x \Delta(x')dx' + ik_y y\right) \tag{8}$$

which are exponentially localized at the boundary and can propagate along it. Find the values of $c_{1,2}$ such that this ansatz solves the Schroedinger equation, and obtain the dispersion relation $E(k_y)$ for these modes. Show that the later describes a *chiral* (i.e. propagating in a single direction) mode.

This simple example known as *Jackiw-Rebbi model* serves as an illustration to the *bulk-to-boundary correspondence*: non-trivial topology (here non-zero Chern numbers) of the *bulk* states (i.e. where $\Delta = \text{const}$) leads to the appearance of the special gapless modes (here a single chiral edge mode) at the *boundary* between two topologically distinct phases.

3 Lattice models in magnetic field: Chern insulators

In this problem we will study one of the possible realizations of *Chern insulators* — a band insulator with non-trivial topological properties of different bands. Consider a two-dimensional tight binding model on a square lattice ($x = ma$ and $y = na$ with $m, n \in \mathbb{Z}$) subject to a perpendicular magnetic field. In the Landau gauge $A_y(x) = Bx$, the hopping matrix elements for links parallel to Oy acquire an x-dependent phase due to the *Peierls substitution*:

$$t_{n,n\pm1}(m) = t_y \cdot \exp\left(i\frac{e}{\hbar c}\int_{n\cdot a}^{(n\pm1)a} A_y(x)dy\right) = t_y \cdot \exp\left(\pm 2\pi i m\Phi/\Phi_0\right) \tag{9}$$

with $\Phi = Ba^2$ and $\Phi_0 = 2\pi\hbar c/e$; so that the corresponding Hamiltonian reads:

$$\hat{H} = -\sum_{m,n}\left(t_x |m-1,n\rangle\langle m,n| + t_y e^{2\pi i m\Phi/\Phi_0}|m,n-1\rangle\langle m,n|\right) + h.c. \tag{10}$$

1. Introduce two *magnetic translation operators*:

$$\hat{T}_x = \sum_{m,n} e^{2\pi i n\Phi/\Phi_0}|m-1,n\rangle\langle m,n|, \quad \hat{T}_y = \sum_{m,n}|m,n-1\rangle\langle m,n| \tag{11}$$

Show by explicit calculation that $\hat{T}_{x,y}^{-1}\hat{H}\hat{T}_{x,y} = \hat{H}$, i.e. $[\hat{T}_{x,y}, \hat{H}] = 0$; but $\hat{T}_y^{-1}\hat{T}_x\hat{T}_y = e^{2\pi i\Phi/\Phi_0}\hat{T}_x \neq \hat{T}_x$, i.e. $[\hat{T}_x, \hat{T}_y] \neq 0$. This means, however, that for rational $\Phi/\Phi_0 = p/q$ with mutually prime $p, q \in \mathbb{Z}$, one has $\hat{T}_y^{-1}\hat{T}_x^q\hat{T}_y = e^{2\pi ip}\hat{T}_x^q = \hat{T}_x^q$ (with $\hat{T}_x^q$ being q-th power of $\hat{T}_x$):

$$[\hat{T}_x^q, \hat{H}] = [\hat{T}_y, \hat{H}] = [\hat{T}_x^q, \hat{T}_y] = 0, \quad \text{for} \quad \Phi/\Phi_0 = p/q, \quad p, q \in \mathbb{Z} \tag{12}$$

2. Obtained set of mutually commuting translation operators allows one to utilize the *Bloch theorem*: the eigenstates of the Hamiltonian can be chosen to be also eigenstates both translation operators denoted as $|k_x, k_y\rangle$:

$$\hat{T}_x^q |k_x, k_y\rangle = e^{iqk_x} |k_x, k_y\rangle, \quad \hat{T}_y |k_x, k_y\rangle = e^{ik_y} |k_x, k_y\rangle, \quad \{qk_x, k_y\} \in [-\pi, \pi], \tag{13}$$

The most general form of the wavefunction which satisfies these two properties is parametrized by q complex amplitudes $\{\psi_a\}_{a=1}^q$ and has following form:

$$|k_x, k_y\rangle = \sum_{a=1}^{q} \psi_a \sum_{m,n} e^{iqk_x m + ik_y n} |a + mq, n\rangle$$

Substitute this ansatz to the Schroedinger equation $\hat{H}|k_x, k_y\rangle = E(k_x, k_y)|k_x, k_y\rangle$ and show that these amplitudes should satisfy the *Harper* equation:

$$-\left(t_x\left(\psi_{a+1} + \psi_{a-1}\right) + 2t_y \cos(k_y + 2\pi a\Phi/\Phi_0)\psi_a\right) = E(k_x, k_y)\psi_a \tag{14}$$

with twisted periodic boundary conditions $\psi_{a+q} \equiv \psi_a e^{iqk_x}$.

3. Let's for simplicity focus on the case $\Phi/\Phi_0 = 1/3$. Then the Harper equation corresponds to the following 3×3 Bloch Hamiltonian:

$$\hat{H}(k_x, k_y) = -\begin{pmatrix} 2t_y \cos(k_y + 2\pi/3) & t_x & t_x e^{-3ik_x} \\ t_x & 2t_y \cos(k_y + 4\pi/3) & t_x \\ t_x e^{3ik_x} & t_x & 2t_y \cos k_y \end{pmatrix} \tag{15}$$

and describes three bands $E_{1,2,3}(k_x, k_y)$. In order to calculate Chern numbers of these bands, we will follow *TKNN (Thouless, Kohmoto, Nightingale, den Nijs)* arguments, which are based on the perturbation theory. We start with the simple case $t_x = 0$: then the bands are k_x-independent and are given trivially by $E_n^{(0)}(k_y) = -2t_y \cos(k_y + 2\pi n/3)$. At which lines of the Brillouin zone these bands intersect?

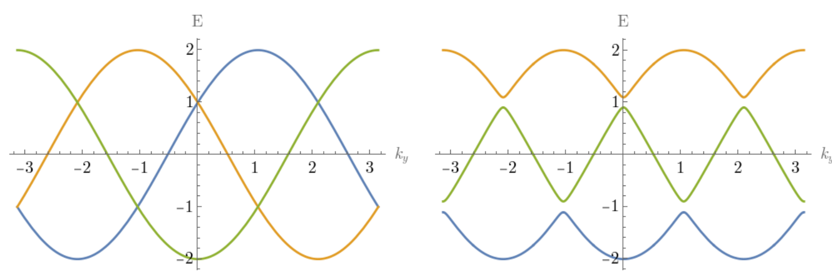

Figure 1: Band structure at $k_x = 0$ for $t_x = 0$ (left) and $t_x \ll t_y$ (right)

4. Introducing small $t_x \ll t_y$ opens gaps at intersections, and the behavior of the Hamiltonian in the vicinity of those points can be obtained by means of the degenerate perturbation theory. In the case of interest, gaps open in the first order which means that it is sufficient to just take corresponding rows and columns of the full Hamiltonian. Moreover, since the Berry curvature involves derivatives of the Hamiltonian w.r.t. both k_x and k_y, only intersection $E_1^{(0)}(k_y) = E_3^{(0)}(k_y)$ will contribute to the Chern numbers. Consider for simplicity the lowest band; then the non-trivial intersection happens around $k_y = -\pi/3$. Show that expansion of the effective Hamiltonian is given by:

$$\hat{H}_{13}(k_x, k_y = -\pi/3 + p_y) \underset{p_y \ll 1}{\approx} -t_y - \begin{pmatrix} -\sqrt{3}t_y p_y & t_x e^{-3ik_x} \\ t_x e^{3ik_x} & \sqrt{3}t_y p_y \end{pmatrix} \tag{16}$$

It describes two branches, upper and lower $E_{\pm}(\boldsymbol{k})$, which corresponds to middle and lowest band in the original problem. Find the Berry curvature, associated with the lowest band:

$$\Omega_{-}(\boldsymbol{k}) = -2\mathrm{Im}\frac{\langle -|\,\partial \hat{H}_{13}(\boldsymbol{k})/\partial k_x\,|+\rangle \langle +|\,\partial \hat{H}_{13}(\boldsymbol{k})/\partial p_y\,|-\rangle}{(E_{+}(\boldsymbol{k}) - E_{-}(\boldsymbol{k}))^2} \tag{17}$$

and obtain the Chern number of the lowest band; the integration over p_y can be expanded to infinity as the integral converges at small momenta $p_y \sim t_x/t_y \ll 1$, while the integration over k_x should be taken over the reduced Brillouin zone $k_x \in [-\pi/q, \pi/q]$:

$$C_{-} \simeq \frac{1}{2\pi}\int_{-\pi/3}^{\pi/3} dk_x \int_{-\infty}^{\infty} dp_y \Omega_{-}(\boldsymbol{k}) \tag{18}$$

The Chern numbers of all remaining bands can be obtained in the same fashion, or obtained by the symmetry considerations: the Chern number of the upper band should be the same, and the sum of Chern numbers of all bands should be zero.

This calculation can be extended to arbitrary flux $\Phi/\Phi_0 = p/q$, although the situation becomes more complicated as coupling between some of the bands occur in higher orders of perturbation theory and slightly more involved analysis is required. It's also not restricted to the limit $t_x \ll t_y$, as it turns out that further increase of t_x won't close the gap and so it cannot change the value of the Chern number, which is a topological invariant.