Institute of Theoretical Physics
University of Cologne

R. Kennedy

Intensive Week "Tools of Topology for Quantum Matter" – Day 1

28.07.2014

Website: `http://www.thp.uni-koeln.de/~rkennedy`

Exercise 1.1. *Chern Insulator*

Consider a two-dimensional square lattice (lattice constant $a = 1$) with Hilbert space $l^2(\mathbb{Z}^2) \otimes \mathbb{C}^2$, realised for example by having two atoms per unit cell. An orthonormal basis of this Hilbert space is given by $\{|x, y, \alpha\rangle\}$, where $(x, y) \in \mathbb{Z}^2$ is the position in the two-dimensional lattice and $\alpha \in \{1, 2\}$.
The Hamiltonian on this lattice is defined by

$$\begin{aligned} H|x, y, \alpha\rangle := \sum_\beta & A_{\alpha\beta}|x + 1, y, \beta\rangle + \overline{A_{\beta\alpha}}|x - 1, y, \beta\rangle \\ & + B_{\alpha\beta}|x, y + 1, \beta\rangle + \overline{B_{\beta\alpha}}|x, y - 1, \beta\rangle \\ & + C_{\alpha\beta}|x, y, \beta\rangle, \end{aligned}$$

where the matrices are given by

$$\begin{aligned} A &:= \frac{1}{2}\left(i\sigma_1 - \sigma_3\right), \\ B &:= \frac{1}{2}\left(i\sigma_2 - \sigma_3\right), \\ C &:= m\sigma_3, \end{aligned}$$

with a parameter $m \in \mathbb{R}$.

a. Change to a basis in which the translation operators are diagonal (i.e. do a Fourier transformation) in order to find the Bloch Hamiltonian $H(k_x, k_y)$.

b. Show that, in general, the Pauli matrices form a basis of the space of traceless 2-by-2 Hamiltonians (the assumption of being traceless neglects constant shifts in energy). Determine the coefficients of $H(k_x, k_y)$ in this basis, i.e. determine the vector $\mathbf{v}(k_x, k_y) \in \mathbb{R}^3$ such that $H(k_x, k_y) = \sum_{i=1}^{3} v_i(k_x, k_y)\sigma_i$.

c. Find the eigenvalues of a general 2-by-2 traceless Hamiltonian. What is the condition for the energy gap to close?

d. Apply the previous result to the Bloch Hamiltonian $H(k_x, k_y)$. For what values of m is the system an insulator?

e. Find the eigenstates of the Bloch Hamiltonian. Is there a choice for the eigenstate with negative eigenvalue that is continuous in k_x and k_y and non-zero everywhere? If yes, under what circumstances? (Math language: When is there a global non-zero section of the bundle?)

f. Show that, in general, the space of Hamiltonians $\tilde{H} : \mathbb{C}^n \to \mathbb{C}^n$ that obey $\tilde{H}^2 = 1$ and have m eigenvalues -1 and $n-m$ eigenvalues $+1$ (socalled "flattened" Hamiltonians) is parameterised by the Grassmannian $\mathrm{Gr}_m(\mathbb{C}^n)$. Deduce that the set of insulator ground state maps $T^d \to \mathrm{Gr}_m(\mathbb{C}^n)$ is equivalent to the set of maps from T^d to the space of flattened Hamiltonians (what is the bijection?). What is the flattened Hamiltonian in the present example?

Mathematica: Part 1

g. Visualise the mapping $(k_x, k_y) \mapsto H(k_x, k_y)$ by identifying $H(k_x, k_y)$ with the vector $\mathbf{v}(k_x, k_y) \in \mathbb{R}^3$. Can you see the torus? Try restricting to only a small, say, k_y-range and subsequently increase to the full range in order to see how the torus is formed.

h. Find the visual representation of what it means for the energy gap to close, i.e. what constitutes the difference between insulator and metal.

i. Compute the Chern number for different values of m.

Exercise 1.2. *Boundaries*

We now introduce boundaries by changing the lattice $\mathbb{Z}^2$ to a strip $\mathbb{Z} \times \mathbb{Z}_L$, for which H is still translation invariant in the x-direction and translation invariance is broken in the y-direction.

a. Use a partial Fourier transform (only in x-direction) in order to arrive at a Bloch Hamiltonian $H(k_x) : \mathbb{C}^{2L} \to \mathbb{C}^{2L}$

Mathematica: Part 2

b. Diagonalise $H(k_x)$ numerically and plot the spectrum as a function of k_x for different values of m. For which values of m is the system insulating?

c. Investigate the states with zero energy by plotting their probability density in the y-direction. What is the average position in y-direction?

Exercise 1.3. *Quantum Spin Hall Effect*

The Quantum Spin Hall Effect is a topological phase realised in quasi two dimensional HgTe quantum wells. The theoretical description of this physical realisation is obtained by augmenting the two band Hilbert space $\mathbb{C}^2$ by a spin degree of freedom to $\mathbb{C}^2_{\text{spin}} \otimes \mathbb{C}^2$. Now there can exist two Chern insulators simultaneously: One for spin up electrons and one for spin down electrons. The difference to the usual Chern insulator is the fact that this combination of two Chern insulators is time reversal invariant. The time-reversal operation $\mathcal{T}$ is defined on operators $A(k) : \mathbb{C}^2_{\text{spin}} \otimes \mathbb{C}^2 \to \mathbb{C}^2_{\text{spin}} \otimes \mathbb{C}^2$ by

$$\mathcal{T} : A(k) \mapsto (\sigma_2 \otimes 1)\overline{A(-k)}(\sigma_2 \otimes 1),$$

where $k = (k_x, k_y)$ in two dimensions.

a. Using two 2-band Bloch Hamiltonians $H_\uparrow(k)$ and $H_\downarrow(k)$ for each spin sector separately gives a total Hamiltonian on $\mathbb{C}^2_{\text{spin}} \otimes \mathbb{C}^2$ of the form $H_\uparrow(k) \oplus H_\downarrow(k)$. If one of them is the Bloch Hamiltonian $H_\uparrow(k) := H(k_x, k_y)$ from exercise 1.1, determine the other, $H_\downarrow(k)$, such that the total Hamiltonian is time reversal invariant.

b. Given a flattened Hamiltonian $\tilde{H}(k_x, k_y)$ of a two dimensional system with any number of bands, the formula for the Chern number reads

$$C = \frac{1}{16\pi i} \iint dk_x dk_y \operatorname{Tr}\big(\tilde{H}(\partial_{k_y}\tilde{H}\partial_{k_x}\tilde{H} - \partial_{k_x}\tilde{H}\partial_{k_y}\tilde{H})\big)$$

Show that this simplifies to the formula for the mapping degree in a 2-band model.

Mathematica: Part 3

c. Compute the Chern number of the new 4-band model determined in exercise 1.3.a. for different values of m.

d. Repeat exercises 1.2.a., b. and c. for this model. Which values of m seem to give a non-trivial topological phase?

e. Add terms to the 4-by-4 Bloch Hamiltonian that are non-zero in the off-diagonal sectors (coupling spin up and down), but which keep it gapped and time reversal invariant. What happens to the gapless states from exercise 1.3.d.? What happens when you break time reversal invariance?