Problem Set 11
Theoretical Solid State Physics (SoSe2017)

No due date

This problem set helps you to read: Liang Fu, C.L. Kane, Time reversal polarization and a Z_2 adiabatic spin pump, Phys. Rev. B **74**, 195312 (2006). The basic point of this paper is to work out the relation between quantum spin Hall insulators and adiabatic pumps. In problem 1, we remind ourselves of the corresponding relation for Chern insulators. This case is described by a Z topological index, the Chern number, while we have already seen in class that the quantum spin Hall effect is described by a Z_2 index. In problem 2, we introduce the concept of Wannier states and show how they are related to the modern theory of polarization. Our discussion here provides an alternative approach to this theory which is reviewed in Sec. IIIA of the paper. Problem 3 and 4 ask you to closely follow discussstions and calculations in the paper.

Problem 1: Punping and Chern insulators

Laughlin's argument provides a direct link between the physics of Chern insulators and adiabatic quantum transport (or, in other words, a quantum pump). This problem is meant to make this relation (yet more) explicit for the square-lattice model of the Chern insulator,

$$H = \tau_x \sin k_x + \tau_y \sin k_y + \tau_z(\Delta + \cos k_x + \cos k_y). \tag{1}$$

Consider this model on a cylinder, rolled up in the y-direction, threaded by a magnetic flux ϕ along the cylinder's axis.

(a) Explain why increasing the flux by a flux quantum ϕ_0 induces the change $k_y \to k_y + 2\pi/L$ where L is the circumference of the cylinder.

(b) Use the theory of adiabatic quantum transport to show that the total charge Q pumped along the cylinder is given by a Chern number when the model is gapped and only the lower band is occupied.

(c) Now consider a one-dimensional pump which is described by the same Hamiltonian, except that now, k_y is taken as a time-dependent parameter which changes by 2π in a time interval T, e.g., from $-\pi$ to π or from 0 to 2π. The latter is implemented by the choice

$$k_y = 2\pi t/T. \tag{2}$$

Assuming the the lower band is fully occupied, show that the total charge pumped along the chain is again given by a Chern number and this Chern number is identical to the one in part (b).

(d) Discuss the explicit amount of charge pumped along the chain in part (c) as a function of the parameter Δ.

Problem 2: Wannier states

Bloch states are delocalized throughout the entire system. Frequently, it is useful to define an orthonormal set of localized basis functions which are based on the Bloch states. Note that the atomic orbitals are not qualifying since the same orbital, but localied on different lattice sites are in general not orthogonal. This motivates the definition of Wannier states.

Start with the Bloch states of a one-dimensional system with N unit cells (of volume 1) and periodic boundary conditions,

$$|\psi_{nk}\rangle = \frac{1}{\sqrt{N}} e^{ikx} |u_{nk}\rangle \tag{3}$$

with nomalization $\langle\psi_{nk}|\psi_{n'k'}\rangle = \delta_{nn'}\delta_{kk'}$ and define the Wannier states

$$|R,n\rangle = \frac{1}{\sqrt{N}} e^{-ikR}|\psi_{nk}\rangle. \tag{4}$$

In general, the Wannier state $|R,n\rangle$ is localized near lattice site R.

(a) First prove the following properties:

- The wavefunction $\langle x|R,n\rangle$ of the Wannier state is only a function of $x-R$ by showing that $\langle x|R,n\rangle = \langle x+R'|R+R',n\rangle$.
- The Bloch states can be expressed in terms of the Wannier states as $|\psi_{nk}\rangle = \frac{1}{\sqrt{N}}\sum_R e^{ikR}|R,n\rangle$.
- Wannier states are orthonormal, $\langle R,n|R',n'\rangle = \delta_{nn'}\delta_{RR'}$.

(b) Show that the dipole moment of the Wannier states can be expressed as

$$P_n = \langle 0,n|x|0,n\rangle = \int \frac{\mathrm{d}k}{2\pi} A_n(k) \tag{5}$$

with the Berry connection $A_n(k) = i\langle u_{nk}|\partial_k u_{nk}\rangle$.

(c) Show that a gauge transformation $|u_{nk}\rangle \to e^{-imk}|u_{nk}\rangle$ with $m \in Z$ changes $P_n \to P_n + m$. As we saw before in class, the polarization of a crystal is defined only up to integers, defining a polarization lattice.

(d) While polarizations are gauge dependent, changes in polarization are physical. Consider a periodic variation of a time-dependent Hamiltonian $H(t)$ with $H(t) = H(t+T)$. Assume that the Hamiltonian describes a gapped system with all bands being either completely occupied or empty. Use the result of (b) to express the adiabatic change in polarization in terms of a (sum of) Chern number(s).

Problem 3: A spin pump

Consider the spin pump discussed by Fu and Kane. In first quantization the Hamiltonian $H = H_0 + V_h + V_h + V_{\text{so}}$ of the one-dimensional tight-binding model involves a term with uniform hopping,

$$H = t_0 \sum_{j;\alpha=\uparrow,\downarrow} |j,\alpha\rangle\langle j+1,\alpha| + \text{h.c.}, \tag{6}$$

a staggered Zeeman field

$$V_h = h_{\text{st}} \sum_{j,\alpha\beta} (-1)^j |j,\alpha\rangle (s^z)_{\alpha\beta} \langle j,\beta|, \tag{7}$$

a staggered hopping term

$$V_t = \Delta t_{\text{st}} \sum_{j,\alpha} (-1)^j |j,\alpha\rangle\langle j+1,\alpha| + \text{h.c.}, \tag{8}$$

as well as a (uniform) spin orbit term

$$V_{\text{so}} = \sum_{j,\alpha\beta} |j,\alpha\rangle i\mathbf{e}\cdot\mathbf{s}_{\alpha\beta}\langle j+1,\beta| + \text{h.c.}, \tag{9}$$

which generally lifts the spin rotation symmetry.

(a) Show that the spin-orbit term is time reversal symmetric and that the staggered Zeeman term breaks time reversal symmetry.

(b) Consider an adiabatic pumping cycle of duration T defined by

$$\Delta t_{\text{st}} = A\cos\frac{2\pi t}{T} \;\; ; \quad h_{\text{st}} = A\sin\frac{2\pi t}{T} \tag{10}$$

Show that the Hamiltonian of the pump is time reversal symmetric for $t = 0$ and $t = T/2$. What does this imply for the instantaneous eigenstates of the Hamiltonian at these times?

(c) For $V_{\rm so} = 0$, write down the corresponding Bloch Hamiltonian H_k for a fixed spin orientation s^z in the form of a general two-band Hamiltonian. Show that in this limit, the model corresponds to two independent SSH Hamiltonians, one for each spin orientation.

(d) By analogy with known results for the SSH chain, discuss the pumping of charge and spin in this limit.

(e) Also write down the spin orbit term in the Bloch Hamiltonian. Note that you now need two sets of Pauli matrices corresponding to sublattices and spin, i.e., the model is really a four-band model.

(f) Discuss the numerical results shown in Fig. 1(b) of the above mentioned paper.

Problem 4: Z2 invariant

Do the calculations of Sec. IIIB in detail. You can treat the Pfaffian at the same level as we did in class (i.e., restricting to the case where the antisymmetric matrices are 2x2 only.)