

Problem 1. Spin and Chern numbers

In this problem, we will compute Chern number for the Hamiltonian

$$H = -\gamma \mathbf{B} \cdot \mathbf{S} \tag{1}$$

for arbitrary spin $s > \frac{1}{2}$ and spin operators \mathbf{S} defined by the commutation relation $[S_i, S_j] = i\epsilon_{ijk}S_k$ where ϵ_{ijk} is the fully anti-symmetric Levi-Civita symbol.

- (a) If $\mathbf{B} = B\hat{\mathbf{z}}$, find the lowest energy H and arbitrary spin s (call it $|\hat{\mathbf{z}}\rangle$).
- (b) We want the solution of H with $\mathbf{B} = B\hat{\mathbf{n}}$ and $\hat{\mathbf{n}} = (\cos\phi \sin\theta, \sin\phi \sin\theta, \cos\theta)$. To do this, we can rotate $H = -\gamma BS_z$ with the operator $U(\theta, \phi) = e^{-i\phi S_z} e^{-i\theta S_y}$. Show that $U(\theta, \phi)S_zU(\theta, \phi)^\dagger = S_x \cos\phi \sin\theta + S_y \sin\phi \sin\theta + S_z \cos\theta$. (*Hint:* It is useful to use the identity $e^{-iA} B e^{iA} = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \underbrace{[A, [A, \dots, [A, B]]]}_{n \text{ commutators}}$ along with $[S_i, S_j] = i\epsilon_{ijk}S_k$.)
- (c) With the eigenstate from (a) and the transformation from (b), argue that the eigenstate of $H = -\gamma \mathbf{B} \cdot \mathbf{S}$ is $|\hat{\mathbf{n}}\rangle = U(\theta, \phi) |\hat{\mathbf{z}}\rangle$.
- (d) While still keeping s unspecified, compute the Berry connections $A_\phi = \langle \hat{\mathbf{n}} | i\partial_\phi \hat{\mathbf{n}} \rangle$, $A_\theta = \langle \hat{\mathbf{n}} | i\partial_\theta \hat{\mathbf{n}} \rangle$ and the Berry curvature $\Omega_{\theta\phi} = \partial_\theta A_\phi - \partial_\phi A_\theta$.
- (e) Compute the full integral over the sphere $\Phi = \int_0^{2\pi} d\phi \int_0^\pi d\theta \Omega_{\theta\phi}$. Using the Chern theorem, we know that this must be an $2\pi C$ for an integer C . What does this tell us about the allowed values of s ?

Problem 2. Current and adiabatic transport

Here we compute the current induced by an adiabatic change of the Hamiltonian and check that it correctly predicts the change in the electric dipole moment.

(a) Using

$$|\psi(t)\rangle = e^{i\alpha(t)} \left[|n\rangle + \dot{\lambda} |\delta n\rangle \right], \quad (2)$$

(recall that $\alpha(t)$ is a combination of geometric phase and dynamic phase), show that the induced change in some arbitrary operator \mathcal{O} is $\langle \mathcal{O} \rangle = 2\dot{\lambda} \operatorname{Re} \langle n | \mathcal{O} | \delta n \rangle$.

(b) Defining the current operator $\mathcal{J} = -e\mathbf{v}$ in terms of the velocity operator \mathbf{v} and using

$$|\delta n\rangle = -i\hbar \sum_{m \neq n} \frac{\langle m | \partial_\lambda n \rangle}{E_n - E_m} |m\rangle, \quad (3)$$

show that

$$\langle \mathcal{J} \rangle = -2e\hbar\dot{\lambda} \operatorname{Im} \sum_{m \neq n} \frac{\langle n | \mathbf{v} | m \rangle \langle m | \partial_\lambda n \rangle}{E_n - E_m}. \quad (4)$$

(c) Using $\mathbf{v} = -\frac{i}{\hbar}[\mathbf{r}, H]$, show that this becomes $\langle \mathcal{J} \rangle = -2e\dot{\lambda} \operatorname{Re} \langle n | \mathbf{r} | \partial_\lambda n \rangle$. [*Hint*: Note that $\langle n | \mathbf{r} | n \rangle \langle n | \partial_\lambda n \rangle$ is pure imaginary (why?).]

(d) Noting that $\langle \mathcal{J} \rangle$ has the interpretation of $d\mathbf{d}/dt$, where $\mathbf{d} = -e\mathbf{r}$ is the dipole operator, and canceling the dt , show that this becomes $\partial_\lambda \langle \mathbf{d} \rangle = -2e \operatorname{Re} \langle n | \mathbf{r} | \partial_\lambda n \rangle = -e\partial_\lambda \langle n | \mathbf{r} | n \rangle$.

Problem 3. Averaging the guessed-at Polarization

In class, we argued that the guess for polarization

$$\mathbf{P}_{\text{guess}} = \frac{1}{V_{\text{cell}}} \int_{\text{cell}} \mathbf{r} \rho(\mathbf{r}) d^3r \quad (5)$$

does not function as a good definition for bulk polarization. Show that this expression vanishes when averaged over all possible locations of the unit cell origin.

Hint: First show that the average is proportional to $\int_{\text{cell}} \int_{\text{cell}} \mathbf{r} \rho(\mathbf{r} - \mathbf{r}') d^3r d^3r'$ where \mathbf{r}' is the shift of the origin of the cell. Then focus on the \mathbf{r}' integral and argue that the result vanishes.

Problem 4. Filling in some Wannier details

In class, we argued for how Wannier functions are related to the polarization. Here we fill in some of the details for one-dimension.

The Wannier functions for band n are defined via

$$|\phi(R)\rangle = a \int_0^{2\pi/a} \frac{dk}{2\pi} e^{ik(R-\hat{r})} |u_{nk}\rangle, \quad (6)$$

for the position operator \hat{r} (over all of space, not just a unit cell). For this problem, it is useful to insert the identity $1 = \int_{-\infty}^{\infty} dr |r\rangle \langle r| = \sum_R \int_0^a dr |R+r\rangle \langle R+r|$ and $R = na$ for an integer n .

(a) Confirm that $\langle \phi(R) | \phi(R) \rangle = 1$.

(b) Show that

$$(\hat{r} - R) |\phi(R)\rangle = -\frac{a}{2\pi} \int_0^{2\pi/a} dk e^{ik(R-\hat{r})} |i\partial_k u_{nk}\rangle. \quad (7)$$

(c) Finally, show that $\langle \phi(R) | (\hat{r} - R) | \phi(R) \rangle = \frac{a}{2\pi} \int_0^{2\pi/a} dk \langle u_{nk} | i\partial_k u_{nk} \rangle = \frac{a}{2\pi} \phi_n$. The polarization is then $P = -e \langle \phi(R) | \hat{r} - R | \phi(R) \rangle$.

Problem 5. Polarization and charge pump

Consider the Hamiltonian whose unit cell includes three sites and is written as

$$H = -t \sum_j (|j\rangle \langle j+1| + \text{h.c.}) - \delta \sum_j \cos(2\pi j/3 - \lambda) |j\rangle \langle j|. \quad (8)$$

In this problem, we will use `pythtb.py` to determine how charge is pumped as we vary λ for each band. Recall from class that the polarization for band n is

$$P_n = -\frac{e}{2\pi} \phi_n, \quad \phi_n = \oint dk A_n(k), \quad (9)$$

and ϕ_n is directly related to the center of Wannier functions as $\bar{x}_n = a\phi_n/(2\pi)$ with lattice spacing a .

- (a) Run the code `chain_3_cycle.py` (see course website). What does the output tell us about the pumped charge and how it is quantized?
- (b) Modify the program to plot the Wannier center positions (Berry phase) of each of the three bands separately, thereby obtaining the cycle Chern number for each band. Before generating plots, ask yourself what you expect. The Wannier center of the lowest-energy band moves to the right during the cycle. Do you expect the same for the highest energy band, or do you expect it to move in the reverse direction? Any guess about the middle band?
- (c) Now make a plot of the pumped charged if the two lowest bands are occupied and if all three bands are occupied.