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Exercise sheet: Aussois GDR Meeetic school

Exercise 1 - Warm-up: completing the results left

(a) Show that the polarization

$$P_n = -\frac{e}{2\pi}\int_0^{2\pi} dk\, \langle u_k^n | i\partial_k | u_k^n \rangle, \tag{1}$$

Changes by an integer unit of the electronic charge, i.e. $P_n \to P_n + em$ with $m \in \mathbb{Z}$ when $|u_k^n\rangle \to e^{-i\phi_k^n}|u_k^n\rangle$.

(b) Show that the Berry curvature $\mathbf{\Omega}_{\mathbf{k}}^n = \partial_{\mathbf{k}} \times \mathbf{A}_{\mathbf{k}}^n$ is a gauge invariant object under the transformation $|u_{\mathbf{k}}^n\rangle \to e^{-i\phi_{\mathbf{k}}^n}|u_{\mathbf{k}}^n\rangle$.

(c) To make the analogy with the electromagnetic field strength, the Berry curvature is sometimes regarded as a two component, anti-symmetric tensor:

$$\Omega_{ij,\mathbf{k}}^n = \partial_{k_i} A_{j,\mathbf{k}}^n - \partial_{k_j} A_{j,\mathbf{k}}^n \tag{2}$$

in terms of $\mathbf{A}_{\mathbf{k}}^n = i\langle u_{\mathbf{k}}^n | \partial_{\mathbf{k}} u_{\mathbf{k}}^n \rangle$. Show that this tensor can be written as

$$\Omega_{ij,\mathbf{k}} = -2\mathrm{Im}\langle \partial_{k_i} u_{\mathbf{k}}^n | \partial_{k_j} u_{\mathbf{k}}^n \rangle \tag{3}$$

Exercise 2 - Quantum spin Hall

Consider the Bernevig-Hughes-Zhang model for CdTe/HgTe quantum wells

$$h_{\mathbf{k}} = \sin k_x \Gamma_1 + \sin k_y \Gamma_2 + M_{\mathbf{k}} \Gamma_0 \tag{4}$$

with $\Gamma_1 = \sigma_z \otimes \tau_x$, $\Gamma_2 = \sigma_0 \otimes \tau_y$ and $\Gamma_0 = \sigma_0 \otimes \tau_z$ 4×4 matrices, and $M_{\mathbf{k}} = 2 - m - \cos k_x - \cos k_y$. The Pauli matrices σ act on spin-space, while the Pauli matrices τ act on orbital space, which we won't specify for now.

(a) Show that $\hat{T} = i\sigma_y \otimes \tau_0 \mathcal{K}$ represents the time-reversal symmetry operator of $h_{\mathbf{k}}$ by computing $\hat{T} h_{\mathbf{k}} \hat{T}^{-1} = h_{-\mathbf{k}}$.

Tip: note that we can act independently on spin and orbital sub-spaces so we can use that $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$ and $\{\tau, \tau_j\} = 2\delta_{ij}$.

(b) Can you guess what could be the inversion operator? Recall that inversion acts as $\hat{I} h_{\mathbf{k}} \hat{I}^{-1} = h_{-\mathbf{k}}$ and that $\hat{I}$ is a unitary operator.

To facilitate the task, we can consider the Hamiltonian is given in the basis defined by

$$\left\{ |p, m_J = \frac{3}{2}\rangle, |s, m_J = \frac{1}{2}\rangle, |p, m_J = -\frac{3}{2}\rangle, |s, m_J = -\frac{1}{2}\rangle \right\}.$$

in terms of s and p orbitals. Can you give a physical reason why $\hat{I}$ has this form?

(c) In class we discussed the Fu-Kane formula [1]

$$\nu = \prod_{n \in \text{occ}} \prod_{\mathbf{k} \in \text{TRIM}} \xi_{\mathbf{k}}^{2n} \tag{5}$$

It allows you to calculate the invariant $\nu = 0, 1$ from the inversion eigenvalues of each occupied eigenstate of a given Kramers-Pair $\xi_{\mathbf{k}}^{2n}$. Here $n \in$ occ labels the occupied bands and TRIM stands for time-reversal invariant momenta, for which $\mathbf{k} = -\mathbf{k}$ up to a lattice vector. Calculate the invariant for different parameters using this invariant as a function of m. How many phases are there and what are their invariants?

(d) The Hall conductivity for this model can be written as

$$\sigma_{xy} = \frac{1}{2}(\sigma_{xy}^{\uparrow} + \sigma_{xy}^{\downarrow}) = \frac{C_{\uparrow} + C_{\downarrow}}{2} \frac{e^2}{h}, \tag{6}$$

where $C_{\uparrow}$ and $C_{\downarrow}$ are the Chern numbers for spin up and spin down subspace of the Hamiltonian. The spin Hall conductivity is determined by the difference between the Hall conductivity of different spin subspaces

$$\sigma_{xy}^{s} = \frac{1}{2}(\sigma_{xy}^{\uparrow} - \sigma_{xy}^{\downarrow}) = \frac{C_{\uparrow} - C_{\downarrow}}{2} \frac{e^2}{h}. \tag{7}$$

Calculate the Hall and spin-Hall conductivity of this model in all phases. Can you give a symmetry argument to justify your result for the Hall conductivity?

Exercise 3 - Low-energy description of a Weyl semimetal

A Weyl Hamiltonian of positive chirality can be defined as:

$$H_+ = +v_f \mathbf{k} \cdot \boldsymbol{\sigma} \tag{8}$$

(a) Write the most general form of a constant perturbation to H_+. Check that it is impossible to gap out such a Weyl Hamiltonian.
Tip: The only perturbations that can be added to H are proportional to the Pauli matrices or the identity.

(b) Check that the Berry curvature takes the form of a monopole in momentum space. Give an argument why Berry monopoles must always come in pairs within the Brillouin zone.
Tip: You may use (or even better, prove!) that the Berry curvature for a two band system $h_k = d_k \cdot \boldsymbol{\sigma} + \varepsilon_k \sigma_0$ is given by [2]

$$\boldsymbol{\Omega}_k = \frac{1}{2}\frac{\mathbf{d}_k}{|d_k|^3}, \tag{9}$$

which can be derived from

$$\Omega_k^i = \frac{\epsilon^{ijl}}{2}\hat{d}_k \cdot (\partial_{k_j}\hat{d}_k \times \partial_{k_l}\hat{d}_k). \tag{10}$$

which we derived in the second lecture.

(c) Double the Hamiltonian with a Weyl of the opposite chirality $H_- = -v_f \mathbf{k} \cdot \boldsymbol{\sigma}$ such that $H = \tau_z \otimes v_f \mathbf{k} \cdot \boldsymbol{\sigma}$ where τ_z is a valley, or orbital degree of freedom. What happens to the spectrum when we add the off-diagonal term $M\tau_x \otimes \sigma_0$?
Tip: Square the Hamiltonian and use to get the eigenvalues.

(d) Add a perturbation of the form $\tau_0 \otimes \mathbf{b} \cdot \boldsymbol{\sigma} + b_0 \tau_z \otimes \sigma_0$. Plot the spectrum for different values of $(\mathbf{b}^2 - b_0^2)/M^2$ and identify the different phases.
Tip: Solve the Hamiltonian numerically in Mathematica, or even better, argue perturbatively.

(e) Show that $\tau_0 \otimes \mathbf{b} \cdot \boldsymbol{\sigma}$ and $b_0 \tau_z \sigma_0 \otimes \tau_0$ break time-reversal $T = -i\sigma_y \mathcal{K} \otimes \tau_0$ and inversion $I = \sigma_0 \otimes \tau_x$, respectively. Show that it is only possible to have Weyl fermions if either, or both symmetries are broken.

Exercise 4 - Lattice model for a Weyl semimetal

Consider the three-dimensional model:

$$H_{\mathbf{k}} = t\sin(k_x)\sigma_x + t\sin(k_y)\sigma_y + (m - t\sum_{i=x,y,z}\cos(k_i))\sigma_z \tag{11}$$

(a) Show that for $m/t = 2$ the gap closes at two points, the Weyl cones, and give their position in momentum space.

(b) Assuming that Pauli's matrices represent a spin degree of freedom, show that this Hamiltonian breaks time-reversal symmetry.
Tip: Time-reversal symmetry is given by $T = -i\sigma_y\mathcal{K}$.

(c) Fix $m/t = 2$ and show that this model has a surface state, known as the Fermi arc, between the two Weyl nodes.
Tip: Check the Chern number as a function of k_z.

(d) Calculate the Hall conductivity σ_{xy}, of this model as a function of the Weyl node separation ΔK_W. What happens when the nodes touch at the Brillouin zone boundaries?
Tip: Use how the Chern number varies as a function of k_z.

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References

[1] L. Fu and C. L. Kane, "Topological insulators with inversion symmetry," *Phys. Rev. B*, vol. 76, p. 045302, Jul 2007.

[2] D. Xiao, M.-C. Chang, and Q. Niu, "Berry phase effects on electronic properties," *Reviews of Modern Physics*, vol. 82, pp. 1959 – 2007, 07 2010.