Les Houches Doctoral School
Exercise Sheet +Solutions

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Two ways to construct a Weyl semimetal

Exercise 1 : Low-energy description of a Weyl semimetal

A Weyl Hamiltonian of positive chirality can be defined as:

$$H_+ = +v_f \mathbf{k} \cdot \boldsymbol{\sigma} \tag{1}$$

(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.

Solution: We can write the most general perturbation as $H_+ = \mathbf{b} \cdot \boldsymbol{\sigma} + b_0\sigma_0$. These perturbations only shift the Weyl point in energy-momentum space. Thus, they can be absorbed in our definition of the origin in momenta and energy, and thus do not open up a gap.

(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 [1]

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

which can be derived from

$$\Omega^i_k = \frac{\epsilon^{ijl}}{2} \hat{d}_k \cdot (\partial_{k_j} \hat{d}_k \times \partial_{k_l} \hat{d}_k). \tag{3}$$

which we derived in the second lecture.

Solution: Since the Hamiltonian is linear in momentum, we can write:

$$\boldsymbol{\Omega}_k = \frac{1}{2}\frac{\mathbf{k}}{|k|^3} = \frac{1}{2}\frac{1}{|k|^2}\hat{e}_r, \tag{4}$$

which is a monopole centred at $k = 0$.

(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 $M\tau_x \otimes \sigma_0$?

Solution: The spectrum gaps out. We can see this by squaring the Hamiltonian:

$$\begin{aligned}
H^2 &= (\tau_z \otimes v_f \mathbf{k} \cdot \boldsymbol{\sigma} + M\tau_x \otimes \sigma_0)^2 && (5)\\
&= (\tau_z \otimes v_f \mathbf{k} \cdot \boldsymbol{\sigma})^2 + (M\tau_x \otimes \sigma_0)^2 && (6)\\
&+ (M\tau_x \otimes \sigma_0)(\tau_z \otimes v_f \mathbf{k} \cdot \boldsymbol{\sigma}) + (\tau_z \otimes v_f \mathbf{k} \cdot \boldsymbol{\sigma})(M\tau_x \otimes \sigma_0) && (7)\\
&= v_f^2(\mathbf{k}^2 + M^2)\tau_0 \otimes \sigma_0 && (8)
\end{aligned}$$

In going form the second to third equality we have used the anti-commutation of the Pauli matrices and the fact that they square to the identity. By taking the square root, the last equality implies that the spectrum is $\epsilon_\pm = \pm\sqrt{\mathbf{k}^2 + M^2}$ which is a gapped Dirac spectrum.

(d) Add a perturbation of the form $\tau_0 \otimes \mathbf{b}\cdot\boldsymbol{\sigma} + b_0\tau_z\sigma_0$. 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.

Solution: For $M^2 \gg (\mathbf{b}^2 - b_0^2) = -b^2$ we have an insulator, since we can connect adiabatically to the limit where $b_\mu = (b_0, \mathbf{b}) = 0$. In general the bands are not degenerate since time-reversal symmetry and inversion are broken by $\mathbf{b}$ and b_0, respectively. For $M^2 \ll -b^2$ the Hamiltonian is connected to the case where $M = 0$. For this case the Hamiltonian is simply:

$$H = (\mathbf{k} - \tau_z\mathbf{b})\tau_z \otimes \boldsymbol{\sigma} + b_0\tau_z\sigma_0 \tag{9}$$

which represents two Weyls sparated in energy by $2b_0$ and in momentum by $2\mathbf{b}$. For the general case, we have two Weyls separated by $2b_\mu\sqrt{1 - M^2/b^2}$, where $b_\mu = (b_0, \mathbf{b})$ and $b^2 = (-b_0^2 + \mathbf{b}^2)$. When the argument of the square root becomes imaginary, the Weyls meet, and we transition to an insulator.
The eigenvalues are given by:

$$E^{s=\pm1}(\mathbf{k}) = \pm\sqrt{(\mathbf{k}\times\hat{b})^2 + \left(|\mathbf{b}| + s\sqrt{m^2 + (\mathbf{k}\cdot\hat{b})^2}\right)^2} \tag{10}$$

For more details, see section 1 in Ref. [2] and [3].

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

Solution: The term proportional to $\mathbf{b}$ can be interpreted as a Zeeman term, and thus breaks time-reversal. We can also do an explicit computation to check that $TH_{-k}T^{-1} \neq H_{-k}$ with $T = -i\sigma_y\mathcal{K}$:

$$\begin{aligned} Th_kT^{-1} &= -i\sigma_y(b^x\sigma_x + b^y\sigma_y + b^z\sigma_z)^* i\sigma_y && (11)\\ &= -b^x\sigma_x - b^y\sigma_y - b^z\sigma_z \neq h_{-k} && (12)\end{aligned}$$

The term proportional to b_0 breaks inversion, as it does not satisfy the inversion symmetry condition. Focusing on that term we have $Ih_kI^{-1} = Ib_0\tau_z\sigma_0I^{-1} = -b_0\tau_z\sigma_0 \neq h_{-k}$ with $I = \tau_x\otimes\sigma_0$.

Time-reversal maps $k \to -k$ without changing chirality. Inversion maps $k \to -k$ but changes chirality. If time-reversal is broken, but you wish to respect inversion you can have two Weyl nodes at the same energy. If you want to respect time-reversal you need at least four Weyl nodes and to break inversion symmetry.

Exercise 2 : Lattice model for a Weyl semimetal

Consider the three-dimensional model:

$$H_{\mathbf{k}} = t\sin(k_x)\sigma_x + t\sin(k_y)\sigma_y + (m - t\sum_i \cos(k_i))\sigma_z \tag{13}$$

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

Solution: The band dispersion is given by $\epsilon_\pm = \pm\sqrt{t^2\sin(k_x)^2 + t^2\sin(k_y)^2 + (2 - t\sum_i \cos(k_i))^2}$. It vanishes when $k_x = k_y = 0$ and $k_z = \pm K_W = \pm\cos^{-1}(0) = \pm\frac{\pi}{2}$, which sets the positions of the nodes.

(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 $T = -i\sigma_y\mathcal{K}$.

Solution: The simplest way to see it is that this model is a Chern insulator model that we studied in the lectures with a mass that varies with k_z. In other words we can write:

$$H_{\mathbf{k}} = H_{CI}(k_x, k_y, M) - t\cos(k_z)\sigma_z = H_{CI}(k_x, k_y, M(k_z)). \tag{14}$$

Since the original Chern insulator model breaks time-reversal symmetry (has a finite Chern number), H has to break TRS too.
Alternatively we can see explicitly that the σ_z term is not invariant under the TRS operator $T = -i\sigma_y\mathcal{K}$. If T represents time-reversal symmetry then $TH_{\mathbf{k}}T^{-1} = H_{\mathbf{k}}$. For any two-band hamiltonian of the form $h_k = d_k \cdot \boldsymbol{\sigma} + \varepsilon_k\sigma_0$, if time-reversal is a symmetry we impose that

$$Th_kT^{-1} = -i\sigma_y(d_k^x\sigma_x + d_k^y\sigma_y + d_k^z\sigma_z + \varepsilon_k\sigma_0)^* i\sigma_y \tag{15}$$

$$= -d_k^x\sigma_x - d_k^y\sigma_y - d_k^z\sigma_z + \varepsilon_k\sigma_0 = d_{-k}\cdot\boldsymbol{\sigma} + \varepsilon_{-k}\sigma_0 \tag{16}$$

which implies that i) $d_k^{x,y,z}$ are odd functions of k, and ii) ε_k is an even function of k. Since condition i) is not satisfied for the z component, our Hamiltonian breaks time-reversal symmetry.

(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.

Solution: For a fixed k_z the Chern number of the Hamiltonian is $C = 1$ between the nodes and $C = 0$ otherwise. This implies that under open boundary conditions in the x or y directions, there is an edge state per k_z. These edge states form the arc.
To see this explicitly note that with these parameters the Weyl nodes sit at $\pm\pi/2$, i.e. there are maximally separated. Thus we can choose $k_z = 0, \pi$ as points between and outside the nodes, and see how the Chern number changes as a function of k_z.
For $H_{k_x,k_y,k_z=0}$, the system is 2D, and realizes a Chern insulator with $M/t = 1$ (M as defined in our second lecture), which falls in $-2 < M/t < 0$ and has $C = 1$.
For $H_{k_x,k_y,k_z=\pi}$ the model is a Chern insulator with $M/t = 3$ which is in the $M/t > 3$ phase with $C = 0$. Upon opening the boundary conditions in x or y there will be an edge state for all k_z's in between the Weyl nodes. A constant energy cut will form an arc, hence the name Fermi arcs.

(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.

Solution: The Hall conductivity is given by the integrated Chern number in k_z.

$$\sigma_{xy} = \int_0^{2\pi} \sigma_{xy}(k_z) \frac{dk_z}{2\pi} = \frac{\Delta K_W}{2\pi} C \frac{e^2}{h} \tag{17}$$

where ΔK_W is the Weyl node separation. The last equality follows from the fact that the only contribution to a finite Hall conductivity comes from the region between the Weyl nodes.

References

[1] 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.

[2] A. G. Grushin, "Common and not so common high-energy theory methods for condensed matter physics," *arXiv e-prints*, p. arXiv:1909.02983, Sept. 2019.

[3] P. Goswami and S. Tewari, "Axionic field theory of $(3+1)$-dimensional weyl semimetals," *Phys. Rev. B*, vol. 88, p. 245107, Dec 2013.