Solid State Physics IV

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Two-level system and Weyl semimetals

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Literature:

- J. Cano *et al.*, Phys. Rev. B **95**, 161306 (2017)
- M. Hirschberger, Ph.D thesis, Princeton University (2017)
- A. Vishwanath, Boulder Summer School Lecture Notes, *Topological Semimetals and Symmetry Protected Topological Phases* (2013)

Recap: Low-energy Hamiltonian of Weyl semimetal

The low-energy Hamiltonian of a Weyl semimetal, as discussed in the last lecture, is a direct sum of individual Weyl points

$$H_{\mathrm{tot}} = \bigoplus_i H_i(\mathbf{k}) \tag{1}$$

$$H_i(\mathbf{k}) = \hbar \sum_{\mu} w_\mu (k_\mu - k_\mu^{(0,i)}) + \hbar \sum_{\mu\nu} (k_\mu - k_\mu^{(0,i)}) A_{\mu\nu} \tau_\nu \tag{2}$$

where w_μ is the tilt vector, $\mathbf{k}^{(0,i)}$ is the 'position' of the Weyl i node in momentum space, $A_{\mu\nu}$ is the velocity matrix, and τ_ν are (pseudospin) Pauli matrices.

We choose the simplest case, $w_\mu = 0$ and $A_\mu \nu = \mathrm{diag}(v, v, v)$, i.e., the band dispersion is isotropic. The simplified Hamiltonian is

$$H_i(\mathbf{k}) = \hbar v (\mathbf{k} - \mathbf{k}^{(0)}) \cdot \boldsymbol{\tau} \tag{3}$$

It may be diagonalized to give the energy dispersion

$$E(\mathbf{k}) = \pm\left|\mathbf{R}(\mathbf{k})\right| = \pm\hbar\left|v\right|\left|\mathbf{k}-\mathbf{k}^{(0,i)}\right| \tag{4}$$

and $\mathbf{R}(\mathbf{k}) = \hbar v(\mathbf{k}-\mathbf{k}^{(0)})$ was defined in analogy to previous sections on Berry curvature in two-level systems.

4.3 Berry curvature of a Weyl point

We consider a single subspace $H_i(\mathbf{k}) = \mathbf{R}(\mathbf{k})\cdot\boldsymbol{\tau}$ while omitting the index i. In a previous section, we have calculated the Berry curvature $\boldsymbol{\Omega}(\mathbf{R}) = \pm\mathbf{R}/(2R^3)$ in $\mathbf{R}$-space. A coordinate transformation to $\mathbf{k}$-space must be carried out carefully, viz.

$$\mathbf{A}(\mathbf{k}) = -i\left\langle n\right|\nabla_{\mathbf{k}}\left|n\right\rangle = -i\left\langle n\right|\frac{\partial\mathbf{R}}{\partial\mathbf{k}}\nabla_{\mathbf{R}}\left|n\right\rangle = (\hbar v)\mathbf{A}(\mathbf{R}) \tag{5}$$

$$\boldsymbol{\Omega}(\mathbf{k}) = \nabla_{\mathbf{k}}\times\mathbf{A}(\mathbf{k}) = \frac{\partial\mathbf{R}}{\partial\mathbf{k}}\nabla_{\mathbf{R}}\times(\hbar v)\mathbf{A}(\mathbf{R}) = (\hbar v)^2\,\boldsymbol{\Omega}(\mathbf{R}) \tag{6}$$

Hence, the Berry curvature in momentum space is

$$\boldsymbol{\Omega}(\mathbf{k}) = \pm\frac{\mathbf{k}-\mathbf{k}^{(0,i)}}{2\left|\mathbf{k}-\mathbf{k}^{(0,i)}\right|^3} \tag{7}$$

4.3.1 Comment on the sign of the Berry curvature of a Weyl point (WP)

When we consider a 2D cut of the Fermi surface at a fixed energy, we can say that the pseudospin, written in terms of eigenfunction spinors such as $(1, 0)$, 'winds around' the WP while pointing radially inward (towards the WP) or outward (away from the WP).

When we change the Fermi energy from hole-like to electron-like, the in/out direction of this pseudospin is reversed. In fact, the sign of the emergent magnetic field is also reversed, but because the sign of the charge is also flipped (hole-like vs. electron-like), the effective Lorentz force in momentum space retains the same sign.

For a unique definition, we now always define the sign of the Berry curvature for Fermi energy above the Weyl point ($E > 0$). In this case, the sign of v — or in the more general anisotropic case, the sign of $\det(A_{\mu\nu})$ — control the sign of the Berry curvature, $\pm$ in Eq. (7).

4.3.2 Chirality of a Weyl point

As noted above, the emergent magnetic field in momentum space is a series of point charges. The chirality of a Weyl point (or topological charge) may be evaluated over a spherical surface like

$$\chi = \int_S \frac{d^2\mathbf{h}}{2\pi} \mathbf{\Omega}(\mathbf{k}) \cdot \hat{\mathbf{n}}(\mathbf{k}) = \pm \int_S \frac{d^2\mathbf{h}}{2\pi} \frac{\mathbf{h}}{2h^3} \cdot \hat{\mathbf{h}} = \pm 1 \tag{8}$$

where $\mathbf{h} = \mathbf{k} - \mathbf{k}^{(0)}$ represents a coordinate shift.

This is the topological invariant associated with the presence of the Weyl point, and cannot be changed in a continuous process (without mutual annihilation of Weyl points). It can be shown that Berry curvature is strictly zero when time reversal and inversion symmetry are enforced simultaneously. Therefore, Weyl points can appear in real materials only if either time or inversion symmetry are broken, or both.

4.3.3 Nielsen-Ninomiya theorem

The low-energy mdel used so far can be extended to a lattice model (tight binding model) in principle. In the lattice model, there can be no net flux through the boundary of the Brillouin zone, due to the periodicity of functions such as $\mathbf{\Omega}(\mathbf{k})$ in momentum space.

When extending the surface integral to the boundary of the Brillouin zone, $\chi = 0$ is thus enforced. This implies, by extension, that Weyl points occur in pairs of opposite chirality in the Brillouin zone.

4.4 Landau quantization of Weyl fermions in a magnetic field

Let us consider the effect of a magnetic field on the Weyl Hamiltonian

$$\mathbf{p} = \hbar\mathbf{k} \rightarrow \mathbf{\Pi} = -i\hbar\nabla - q\mathbf{A} \tag{9}$$

$$H = v(-i\hbar\nabla - q\mathbf{A}) \cdot \boldsymbol{\tau} \tag{10}$$

where $\mathbf{A} = (0, Bx, 0)^T$ is the electromagnetic vector potential in our chosen gauge, giving uniform B with $\mathbf{B} \parallel \hat{z}$. The commutators for the canoncical momentum can be derived explicitly by using $[\partial_x, x] = 1$ and

$$[\Pi_x, \Pi_y] = i\hbar qB \tag{11}$$

Raising and lowering operators may be derived from these via

$$a = \frac{l_B}{\hbar\sqrt{2}}\left(\Pi_x + is\Pi_y\right) \tag{12}$$

$$a^\dagger = \frac{l_B}{\hbar\sqrt{2}}\left(\Pi_x - is\Pi_y\right) \tag{13}$$

and $l_B = \sqrt{\hbar/(qB)}$ is the magnetic length and $s = \mathrm{sgn}(qB)$. This definition enforces

$$[a, a^\dagger] = \frac{l_B^2}{2\hbar^2}\left([-\Pi_x, is\Pi_y] + [is\Pi_y, \Pi_x]\right) = \frac{1}{2\hbar\,|qB|}(-i\cdot i)\hbar qB\cdot 2s = +1 \tag{14}$$

as required for the bosonic commutators (we will proceed with bosonic quantization in a harmonic oscillator scheme).

The Hamiltonian reads in second quantization

$$H = v\begin{pmatrix} \Pi_z & \Pi_x - i\Pi_y \\ \Pi_x + i\Pi_y & -\Pi_z \end{pmatrix} \to v\begin{pmatrix} \hbar k_z & \frac{\hbar\sqrt{2}}{l_B}a \\ \frac{\hbar\sqrt{2}}{l_B}a^\dagger & -\hbar k_z \end{pmatrix} \tag{15}$$

where the second step is correct for $s < 0$ — suitable for $B > 0$, $q = -e$ for electrons, where $e > 0$ is the fundamental charge. It also requires assuming plane-wave behavior along the z-axis, i.e. separating the wavefunction into

$$\psi_m(\mathbf{r}) = \exp(ik_z z)\begin{pmatrix} u_1^{(m)}(x,y) \\ u_2^{(m)}(x,y) \end{pmatrix} \tag{16}$$

with harmonic oscillator eigenfunctions obeying

$$a u_i^{(m)} = \sqrt{m}\, u_i^{(m-1)} \tag{17}$$

$$a^\dagger u_i^{(m)} = \sqrt{m+1}\, u_i^{(m+1)} \tag{18}$$

for $i = 1, 2$.

How to diagonalize this 2×2 matrix? First write out Schroedinger's equation explicitly, while introducing $p_z = \hbar k_z$ and $\beta = \frac{\hbar\sqrt{2}}{l_B}$:

$$p_z u_1^{(m)} + \beta a u_2^{(m)} = \frac{E}{v} u_1^{(m)} \tag{19}$$

$$\beta a^\dagger u_1^{(m)} - p_z u_2^{(m)} = \frac{E}{v} u_2^{(m)} \tag{20}$$

This means we require a relation like

$$u_1^{(m)} = A_m u_2^{(m-1)} \tag{21}$$

with a scaling factor A_m. In particular, this implies $u_1^{(0)} = 0$, because anyway $a\, u_2^{(0)} = 0$ must be valid.

Solution for $m \neq 0$: We may write

$$H\psi = v \begin{pmatrix} p_z & \beta a \\ \beta a^\dagger & -p_z \end{pmatrix} \begin{pmatrix} A_m u_2^{(m-1)} \\ u_2^{(m)} \end{pmatrix} = E_m \begin{pmatrix} A_m u_2^{(m-1)} \\ u_2^{(m)} \end{pmatrix} \tag{22}$$

which gives two equations

$$A_m \left(\frac{E_m}{v} - p_z \right) = \beta \sqrt{m} \tag{23}$$

$$A_m \left(\beta \sqrt{m} \right) = \frac{E_m}{v} + p_z \tag{24}$$

which, after eliminating A_m, results in the two solutions

$$E_m = \pm \hbar \, |v| \left(\frac{2m}{l_B^2} + k_z^2 \right)^{1/2} \tag{25}$$

Solution for $m = 0$: Let us consider the case of $m = 0$ where $\psi_0 = \exp(ik_z z)(0, u_2^{(0)})^T$ and

$$H\psi = v \begin{pmatrix} p_z & \beta a \\ \beta a^\dagger & -p_z \end{pmatrix} \begin{pmatrix} 0 \\ u_2^{(0)} \end{pmatrix} = E_0 \begin{pmatrix} 0 \\ u_2^{(0)} \end{pmatrix} \tag{26}$$

which results in a single equation $0 - v p_z u_2^{(0)} = E_0 u_2^{(0)}$ with a single ground state energy

$$E_0 = -\hbar v k_z, \tag{27}$$

where the sign of the velocity v (and hence, the chirality of the Weyl point) directly enters the expression for the energy dispersion.

Discussion: The quantum limit is obtained when only the $m = 0$ Landau level is occupied (note that the degeneracy of Landau levels increases with field). In the quantum limit, the direction of motion of electrons is coupled to the chirality of their Weyl subspace $\chi = \mathbf{B} \cdot \mathbf{v} / (|\mathbf{B}| \cdot |\mathbf{v}|)$, because the $m = 0$ Landau level has a linear dispersion and acts, effectively, like a one-dimensional transport channel. Hence, it is said that Weyl fermions have a chiral $m = 0$ Landau level.

Comaprison to the case of quadratic bands: e.g. in GaAs or Si, we have

$$E = \left(m + \frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m^*} \tag{28}$$

with $\omega_c = qB/m^*$. In the case of a quadratic band and for the linear band with $m > 0$, the dispersion is independent of k_x, k_y because of confinement of motion to Landau tubes. In the lowest Landau level of the linear band ($m = 0$), however, the behavior is akin to the quantum oscillations of a point-like Fermi surface: The Landau tube picture loses its meaning and the transport properties are those of an effective 1D wire.

4.5 Chiral anomaly of Weyl electrons

In the quantum limit, right- or left-moving electrons have to cross a large distance in momentum space to reverse their momentum in a scattering process. We assign an inter-valley relaxation lifetime τ_b to this process, which is large so that the $m = 0$ Landau level becomes a very good conductor.

Consider the kinetic equation

$$\hbar\dot{\mathbf{k}} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \tag{29}$$

and integrate to obtain the corresponding shift of the Fermi surface in steady state

$$\Delta k_z = \frac{q}{\hbar}\, E_z \tau_b \tag{30}$$

We want to calculate the the current density $j = I/A_z = N_c v/A_z$ where I is the charge current, A_z is the sample cross-section perpendicular to the applied magnetic field $\mathbf{B} \parallel \hat{z}$, N_c is the number of carriers involved in the process, E_z is the component of the electric field applied parallel to the z-axis, and q is the charge of particles involved.

To estimate $N_c = \mathcal{D} \cdot g_{1D}(E) \cdot \Delta E$ where

$$\mathcal{D} = \frac{\Phi}{\phi_0} = \frac{BA_z}{h/q} \tag{31}$$

$$g_{1D}(E) = \frac{1}{2\pi}\,\frac{1}{\hbar v} \tag{32}$$

$$\Delta E = \hbar v \Delta k_z = \hbar v \frac{q}{\hbar}\, E_z \tau_b \tag{33}$$

are the degeneracy of Landau levels, the density of states of a 1D electron gas with dispersion $E = \hbar v k$, and ΔE is the energy shift due to the electric field. Taken together,

$$j = \frac{v}{A_z} \frac{1}{2\pi\hbar v} (\hbar v) \left(\frac{q}{\hbar} E_z \tau_b \right) \frac{B A_z}{h/q} = \frac{v q^2 \tau_b}{4\pi^2 \hbar^2} (\mathbf{E} \cdot \mathbf{B}) \tag{34}$$

i.e. the conductivity is strongly dependent on the angle between electric field and the external magnetic field, with a strong enhancement when the two are coaligned and current can flow along the quasi one-dimensional channel provided by the $m = 0$ Landau level.

The $\mathbf{E} \cdot \mathbf{B}$ law for electronic transport due to Weyl fermions may also be derived, in the limit of low magnetic field, from Berry curvature considerations using semiclassical transport theory: Son & Spivak, Phys. Rev. B **88**, 104412 (2013).