

Condensed Matter Physics IV

Lecture 3

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Berry phase of a 2-level system; Weyl semimetal

The University of Tokyo

Max Hirschberger

hirschberger@ap.t.u-tokyo.ac.jp

<http://www.qpec.t.u-tokyo.ac.jp/hirschberger/>

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3.1 Berry phase of a 2-level system (spin-1/2 particle)

Our motivation is:

1. Derivation of quantization conditions without explicitly demanding single-valued wavefunction.
2. Geometric phase calculation shows that we need to rotate a spin *twice* to return to itself.
3. Compare case of spin-1/2 and magnetic monopole: in Aharonov-Bohm effect, we can turn off the magnetic field; in spin-1/2 case, the effective magnetic field is "built-in" and cannot be "turned off".

The general expression for a two-level Hamiltonian (2×2 matrix) is

$$\hat{\mathcal{H}} = R_0 \sigma_0 + \mathbf{R} \cdot \boldsymbol{\sigma} \quad (1)$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ and

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (2)$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (3)$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (4)$$

$$(5)$$

are the Pauli matrices. In spherical coordinates for $\mathbf{R}$, the Hamiltonian can be written as

$$\hat{\mathcal{H}} = \begin{pmatrix} R_z & R_x - iR_y \\ R_x + iR_y & -R_z \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta e^{-i\varphi} \\ \sin \theta e^{+i\varphi} & -\cos \theta \end{pmatrix} \quad (6)$$

and the eigenenergies are

$$E_{\pm} = R_0 \pm |\mathbf{R}| = \pm 1 \quad (7)$$

if $\mathbf{R}$ is normalized to length 1. The eigenfunctions are

$$|n, \mathbf{R}\rangle = |\pm, \mathbf{R}\rangle \quad (8)$$

$$|+, \mathbf{R}\rangle = e^{-i\alpha/2} \begin{pmatrix} e^{-i\varphi/2} \cos(\theta/2) \\ e^{+i\varphi/2} \sin(\theta/2) \end{pmatrix} \quad (9)$$

$$|-, \mathbf{R}\rangle = e^{-i\alpha/2} \begin{pmatrix} -e^{-i\varphi/2} \sin(\theta/2) \\ e^{+i\varphi/2} \cos(\theta/2) \end{pmatrix} \quad (10)$$

These two states are orthonormal and, e.g. at $\theta = 0$, $\varphi = 0$ we have $|+, \mathbf{R}\rangle = e^{-i\alpha/2}(1, 0)^T$ and $|-, \mathbf{R}\rangle = e^{-i\alpha/2}(0, 1)^T$.

At $\theta = \pi/2$, $\varphi = 0$ with $\cos(\pi/4) = \sin(\pi/4) = 1/\sqrt{2}$ we have $|+, \mathbf{R}\rangle = e^{-i\alpha/2} \frac{1}{\sqrt{2}}(1, 1)^T$ and $|-, \mathbf{R}\rangle = e^{-i\alpha/2} \frac{1}{\sqrt{2}}(1, -1)^T$.

3.1.1 Gauge Transformation for Bloch Spinors

A gauge transformation acts as

$$|n\rangle \rightarrow |n'\rangle = U(\theta, \varphi) |n\rangle,$$

where U is a unitary matrix such that $U^\dagger U = \mathbb{I}$ and $U \in SU(2)$.

For example, the unitary matrix describing rotations around the z -axis is

$$U_z = \exp\left(i\frac{\eta}{2}\sigma_z\right) = \begin{pmatrix} e^{i\eta/2} & 0 \\ 0 & e^{-i\eta/2} \end{pmatrix}.$$

We focus here on a simple – quasi- $U(1)$ – unitary transformation:

$$U = \exp\left(i\frac{\eta}{2}\sigma_z\right) = \begin{pmatrix} e^{i\eta/2} & 0 \\ 0 & e^{-i\eta/2} \end{pmatrix} = e^{i\eta/2\sigma_z}.$$

The Berry connection for this gauge transformation is

$$\mathbf{A}_n \rightarrow \mathbf{A}'_n = -i \langle n' | \nabla_{\mathbf{R}} | n' \rangle = -i \langle n | U^\dagger \nabla_{\mathbf{R}} U | n \rangle = -i \langle n | U^\dagger (\nabla_{\mathbf{R}} U) | n \rangle - i \langle n | \nabla_{\mathbf{R}} | n \rangle.$$

Thus, for the explicit wavefunctions $|\pm, \mathbf{R}\rangle$,

$$\mathbf{A}_+(\mathbf{R}) = -i \langle + | \nabla_{\mathbf{R}} | + \rangle = -\frac{1}{2} [(\nabla \alpha) + (\cos \theta) \nabla \varphi],$$

$$\mathbf{A}_-(\mathbf{R}) = -i \langle - | \nabla_{\mathbf{R}} | - \rangle = -\frac{1}{2} [(\nabla\alpha) - (\cos\theta)\nabla\varphi].$$

In spherical coordinates:

$$\nabla\varphi = \frac{\partial\varphi}{\partial r} \hat{\mathbf{e}}_r + \frac{1}{r} \frac{\partial\varphi}{\partial\theta} \hat{\mathbf{e}}_\theta + \frac{1}{r \sin\theta} \frac{\partial\varphi}{\partial\varphi} \hat{\mathbf{e}}_\varphi = \frac{1}{r \sin\theta} \hat{\mathbf{e}}_\varphi.$$

Therefore,

$$\mathbf{A}_+(\mathbf{R}) = -\frac{1}{2} \left[(\nabla\alpha) + \frac{\cos\theta}{R \sin\theta} \hat{\mathbf{e}}_\varphi \right], \quad \mathbf{A}_-(\mathbf{R}) = -\frac{1}{2} \left[(\nabla\alpha) - \frac{\cos\theta}{R \sin\theta} \hat{\mathbf{e}}_\varphi \right].$$

The overall phase α is a scalar function of θ, φ and can be adjusted by a gauge transformation.

However,

1. Focusing on $|+\rangle$, there is no single gauge where $\mathbf{A}_+(\mathbf{R})$ is well-behaved everywhere.
2. Even if we choose a gauge where $\mathbf{A}_+(\mathbf{R})$ is regular at the north pole, then $\mathbf{A}_-(\mathbf{R})$ is singular at the north pole, and vice versa.

Hence, we define the vector potentials in two gauges:

Label	α	Vector Potential
A_+^N	$-\varphi$	$\frac{1 - \cos\theta}{2R \sin\theta} \hat{\mathbf{e}}_\varphi$
A_+^S	$+\varphi$	$\frac{-1 - \cos\theta}{2R \sin\theta} \hat{\mathbf{e}}_\varphi$
A_-^N	$+\varphi$	$\frac{-1 + \cos\theta}{2R \sin\theta} \hat{\mathbf{e}}_\varphi$
A_-^S	$-\varphi$	$\frac{+1 + \cos\theta}{2R \sin\theta} \hat{\mathbf{e}}_\varphi$

The superscripts N, S denote the north and south pole gauge patches respectively.

We now compute the Berry curvature by taking the curl:

$$\boldsymbol{\Omega}_\pm(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathbf{A}_\pm(\mathbf{R}) = \pm \frac{1}{2} \frac{\mathbf{R}}{|\mathbf{R}|^3}.$$

This has the same form as the field of a *Dirac monopole*, but the charge depends on the spinor state ($|+\rangle$ or $|-\rangle$).

$$\boldsymbol{\Omega}_+(\mathbf{R}) = +\frac{1}{2} \frac{\mathbf{R}}{R^3}, \quad \boldsymbol{\Omega}_-(\mathbf{R}) = -\frac{1}{2} \frac{\mathbf{R}}{R^3}.$$

Note that the emergent magnetic field diverges at $R = 0$, where the assumption of singly degenerate quantum states breaks down in our theory.

3.1.2 Physical Meaning of this emergent magnetic field?

The Berry curvature can be viewed as an emergent magnetic field in parameter space. A movement of the quantum state in parameter space corresponds to an adiabatic rotation of $\mathbf{R}$, akin to the slow rotation of an external magnetic field $\mathbf{B}$ and the Zeeman effect of a spin for the Zeeman Hamiltonian $\hat{H} = \mathbf{H} \cdot \boldsymbol{\sigma}$.

We calculate the geometric phase on a closed loop $\mathcal{C}$ in parameter space:

$$\gamma_{\pm} = \oint_{\mathcal{C}} d\mathbf{l}_{\mathbf{R}} \cdot \mathbf{A}_{\pm}^N(\mathbf{R}) = \int d^2\mathbf{R} \, \hat{\mathbf{n}} \cdot \boldsymbol{\Omega}_{\pm}^N(\mathbf{R}) = \pm\pi \pmod{2\pi}.$$

where we choose the north pole gauge arbitrarily. The last equality requires that the vector potential is regular on the entire surface of integration.

Comments

1. Two full rotations are required for the spinor to return to itself.
2. This result is derived without requiring a single-valued wavefunction; instead, the Berry phase formalism naturally accounts for the spinor's double-valuedness (unlike the $U(1)$ case of the Dirac monopole).
3. Note the difference between $U(1)$ and $SU(2)$ structures of the Hilbert space.
4. For spin-1 (bosons), the geometric phase becomes $\gamma_{\pm}(\mathcal{C}) = 2\pi \pmod{2\pi}$, meaning the wavefunction is single-valued.
5. The geometry is intrinsic to Hilbert space. No external magnetic field is required, unlike in the case of the Aharonov-Bohm effect.

4 Weyl Semimetals

Literature:

- J. Cano *et al.*, *Phys. Rev. B* **95**, 161306 (2017)
- A. Vishwanath, *Lecture Notes, Boulder Summer School* (2013)

4.1 Hamiltonian and General Considerations

We discuss physical consequences of Berry curvature (Hall effect) and bulk–boundary correspondence (surface states) using a “minimal example” — a Weyl semimetal, i.e. a fermion in 3D with linear $\varepsilon\text{--}\mathbf{k}$ dispersion, analogous to 2D graphene.

Minimal Hamiltonian: The low-energy electronic structure near the Fermi energy ε_F is described by

$$H_{\text{tot}} = \bigoplus_i H_i(\mathbf{k}),$$

with

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

where τ_{ν} are the Pauli matrices representing spin or pseudospin degrees of freedom, w_{μ} is the tilt vector, and the components of the velocity matrix are $A_{\mu\nu}$.

In some coordinate frame, $A_{\mu\nu}$ can be chosen to be diagonal:

$$A = \begin{pmatrix} v_x & 0 & 0 \\ 0 & v_y & 0 \\ 0 & 0 & v_z \end{pmatrix}.$$

However, in general, the tilt vector is not along one of the primary axes A .

4.2 Examples and Classification

Three typical cases are sketched in the lecture (qualitatively):

- **Type-I Weyl:** Zero tilt, isotropic velocity. The Fermi surface at $\varepsilon_F = 0$ shrinks to a point (Dirac cone).
- **Anisotropic Type-I:** No tilt but anisotropic velocities, as in real materials such as TaAs or GdPtBi.

- **Type-II Weyl:** Tilt larger than a critical value, leading to electron and hole pockets coexisting at ε_F .

Reference: A. Soluyanov *et al.*, *Nature* **527**, 495 (2015).

4.3 3D Weyl semimetal is robust to perturbations

The *topological invariant* of a Weyl semimetal is the *chirality* (or topological charge) of each Weyl node, defined via the Berry curvature. This quantity is robust to deformations of the electronic structure, disorder, and small perturbations.

For the simplest case:

$$\mathbf{w} = 0 \quad (\text{zero tilt}), \quad A_{\mu\nu} = \text{diag}(v, v, v).$$

Then

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

which diagonalizes to

$$E(\mathbf{k}) = R_0 \pm |\mathbf{R}| = \pm \hbar |v| |\mathbf{k} - \mathbf{k}_i^0|.$$

The sign of v does not matter for the energy bands themselves, but it is important for the character of the wavefunction and it determines whether the Weyl node has right-handed or left-handed chirality.

Hence, the dispersion is *gapless* — there is no separation between conduction and valence bands at $\mathbf{k} = 0$.

This gapless nature is robust against perturbations only in three dimensions.

A general perturbation can be written as

$$H'(\mathbf{k}) = \boldsymbol{\mathcal{E}}(\mathbf{k}) \cdot \boldsymbol{\tau} + \varepsilon_0 \mathbb{I},$$

where we may expand $\boldsymbol{\mathcal{E}}(\mathbf{k}) \approx \boldsymbol{\mathcal{E}}_0 + \dots$ near the Weyl point.

This leads to a shift of the Weyl node position $\mathbf{k}_0^{(i)}$ and an overall energy offset, but no opening of a gap.

Comparison to 2D (graphene)

In two dimensions, $\boldsymbol{\mathcal{E}}$ has more independent vector components than $\mathbf{k}_0^{(i)}$, so certain perturbations (e.g. $\mathcal{E}_z \tau_z$) cannot be absorbed by a simple coordinate shift.

Hence, graphene opens a small gap due to spin-orbit coupling.