Notes of Chapter 2 of Bernevig's Book

Taper

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Abstract

Since I have already made a written one, this note is only an outline of the written script, in the hope of makeing it easier to read.

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1 Deriving Berry Phase

From page 1 to page 2 (equation 2.7), one derives the expression for the phase $e^{i\gamma_m}$ using instaneous energy eigenstate for E_m :

$$H(\vec{R})|n(\vec{R})\rangle = E_m(\vec{R})|n(\vec{R})\rangle \tag{1.0.1}$$

$$\gamma_m = i \int_0^t \langle m \left(\vec{R}(t') \right) | \frac{\partial}{\partial t} m \left(\vec{R}(t') \right) dt' \rangle$$
 (1.0.2)

Then I writes about different ways to get the γ_m :

$$\gamma_m = i \int_{\text{curve}} \langle m | \nabla_{\vec{R}} m \rangle \, d\vec{R} = \int_{\text{curve}} \vec{A}_n \cdot d\vec{R}$$
 (1.0.3)

(equation 2.8) where one defines

Definition 1.1 (Berry Connection, Berry Vector Potential \vec{A}).

$$\vec{A}_n \equiv i \langle n | \nabla_{\vec{R}} \, n \rangle \tag{1.0.4}$$

Then I proves several facts:

Fact 1.1. γ_n is real

By virtue of fact 1.1, we have

$$\gamma_n = -\operatorname{Im} \int_{\text{curve}} \langle n | \nabla_{\vec{R}} \, n \rangle \cdot d\vec{R}$$
 (1.0.5)

Fact 1.2. Berry connection \vec{A}_n is gauge-dependent. The dependence is: If

$$|n\rangle \to |n'\rangle = e^{i\xi(\vec{R})} |n\rangle$$

then

$$\vec{A}_n \to \vec{A}_n - \nabla_{\vec{R}} \, \xi(\vec{R}) \tag{1.0.6}$$

Therefore we have

Fact 1.3. γ_n is gauge-dependent, unless the path transverses a closed loop. Since

$$\gamma_n \to \gamma_n - \left(\xi(\vec{R}(T)) - \xi(\vec{R}(0))\right)$$

It is unchanged unless the integration curve is a closed loop. In which case

$$\xi(\vec{R}(T)) - \xi(\vec{R}(0)) = 2\pi m \stackrel{mod\ 2\pi}{=} 0$$

Example 1.1. There is a simple example on page 3 to show that the Berry phase can be actually detected.

When the parameter space is \mathbb{R}^3 , we have a simpler expression for berry phase. It is derived on page 4 (equation 2.12) that

$$\gamma_n = -\operatorname{Im} \oint \langle \nabla_{\mathbf{R}} n | \times | \nabla_{\mathbf{R}} n \rangle \cdot d\mathbf{s} = -\operatorname{Im} \oint \mathcal{A}^n \cdot d\mathbf{s}$$
 (1.0.7)

where we have defined:

Definition 1.2 (Berry Curvature A^n).

$$A^{n} = \langle \nabla_{\mathbf{R}} n | \times | \nabla_{\mathbf{R}} n \rangle \tag{1.0.8}$$

In components (repeated index automatically summed):

$$\mathcal{A}_{i}^{n} = \varepsilon_{ijk} \left\langle \partial_{i} n | \partial_{k} n \right\rangle \tag{1.0.9}$$

By analogy with the theory of electromagnetic fields, this is also called Berry field, dentoed by F_{jk} in Bernevig's book. More specifically: $F_{jk} = \langle \partial_j n(\mathbf{R}) | \partial_j n(\mathbf{R}) \rangle - (j \leftrightarrow k)$.

2 Gauge-independent calculation of Berry Curvature

For numerical considerations, we Bernevig gives a new way to calculate the Berry curvature. I shows in page 5 to 6 that:

$$\gamma_{n} = -\operatorname{Im} \oint d\mathbf{s} \sum_{m \neq n} \frac{\langle n(\mathbf{R}) | \nabla_{\mathbf{R}} H | m(\mathbf{R}) \rangle \times \langle m(\mathbf{R}) | \nabla_{\mathbf{R}} H | n(\mathbf{R}) \rangle}{(E_{n} - E_{m})^{2}}$$
(2.0.10)

There are two advantages of this formula:

- 1. It is intrinsically gauge-independent (see page 6 for explanation).
- 2. It is no longer necessary to pick $|n\rangle$ to be smooth & single-valued.

Don't know why

There are several remarks about this formula on page 7. One important remark is that:

Fact 2.1.

$$\sum_{n} \gamma_n = 0 \tag{2.0.11}$$

3 Degeneracy and level-crossing

Page 7 has a discussion about the serious problems posed by the degenracy points. Then we turn our attention to two-level system.

3.1 Two-level system and Berry connection A_n

Here Bernevig considers a system with Hamiltonian

$$H = \epsilon(\mathbf{R})I + \mathbf{d}(\mathbf{R}) \cdot \sigma \tag{3.1.1}$$

He first calculate in a general setting and concludes that the Berry field is

$$\mathbf{V}_{-} = \frac{1}{2} \frac{\mathbf{d}}{d^3} \tag{3.1.2}$$

However, I don't think it is a good calculation, explained in page 8. On the other hand, Bernevig also gives an alternative calculation in the following.

3.1.1 Two-level system using Hamiltonian approach

On page 8 to 10, I gives the calculation of Berry phase of Spin in a varying magnetic environment. Consider the Hamiltonian:

$$H(\mathbf{B}) = \mathbf{B} \cdot \mathbf{S} \tag{3.1.3}$$

with

$$n = -s, -s + 1, \cdots, s$$
 (3.1.4)

One finds:

$$\gamma_n = -n \oint \frac{\mathbf{B}}{B^3} \mathrm{d}\mathbf{s} \tag{3.1.5}$$

(equation 2.31) If the integration is taken on the surface of a sphere, then we have (noting that the solid angle $d\Omega = \sin(\theta)d\theta d\phi$. Use Ω to denote the solid angle of the integration area)

$$e^{i\gamma_n} = e^{-in\Omega} \tag{3.1.6}$$

There are several remarks on page 10. The important ones are

Remark 3.1. If we integrate in a whole sphere, and the sphere contains several "poles" - the degeneracy point, we have

$$|\gamma_i| = 4\pi n \times (number\ of\ poles\ inside)$$
 (3.1.7)

Similary, if the paremeter space in 2 dimensional, then

$$|\gamma_i| = 2\pi n \times (number\ of\ poles\ inside)$$
 (3.1.8)

Specifically, for electrons

$$|\gamma_i| = \pi \times (number\ of\ poles\ inside)$$
 (3.1.9)

Therefore, an electron transversing a circle will accumulate a phase of $e^{i\pi}=-1$.

4 Anchor

References

[1] Bernevig's Topological Insulators and Superconductors

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