Lecture notes on topological insulators

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CONTENTS

I. REVIEW OF BERRY PHASE

We first review the **Berry phase** (also known as the **geometric phase**) for a *non-degenerate* energy level (**Abelian** case). The Berry phase for *degenerate* energy levels (**non-Abelian** case) is discussed in the second part.

Note: For the rest of the lecture notes, a matrix is written in the San-serif font, $\mathsf{M} = (M_{\alpha\beta})$.

A. Non-degenerate energy level

Consider a system that varies slowly with parameters $\boldsymbol{\lambda}(t)$. One example is a spin in a slowly varying magnetic field $\mathbf{B}(t)$. At each instant t, the time-independent Schrödinger equation is

$$H_{\boldsymbol{\lambda}}|n,\boldsymbol{\lambda}\rangle = \varepsilon_{n\boldsymbol{\lambda}}|n,\boldsymbol{\lambda}\rangle. \tag{1.1}$$

The eigenstates $|n,\boldsymbol{\lambda}\rangle$ will be called **snapshot states**. We are allowed to assign a $\boldsymbol{\lambda}$-dependent phase $\chi_n(\boldsymbol{\lambda}(t))$ to the snapshot state $|n,\boldsymbol{\lambda}(t)\rangle$, since the new state $e^{i\chi_n(t)}|n,\boldsymbol{\lambda}\rangle$ still satisfies Eq. (1.1).

Suppose energy level $\varepsilon_{n\boldsymbol{\lambda}}$ is gapped from other levels with a minimal separation Δ_0 during the course of evolution, and the characteristic frequency of the changing parameter $\Omega_0 \ll \Delta_0/\hbar$, then according to the **quantum adiabatic theorem**, an initial state $|n,\boldsymbol{\lambda}(0)\rangle$ would stay at the same level n (Fig. 1). After time t, it evolves to the snapshot state at $\boldsymbol{\lambda}(t)$, multiplied by a *dynamical* phase factor,

$$|n,\boldsymbol{\lambda}_0\rangle \to |\Psi_{n\boldsymbol{\lambda}}(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t dt'\varepsilon_{n\boldsymbol{\lambda}(t')}}|n,\boldsymbol{\lambda}(t)\rangle. \tag{1.2}$$

Furthermore, it is possible to develop a $\boldsymbol{\lambda}$-dependent phase $\gamma_n(\boldsymbol{\lambda}(t))$, hence in general,

$$|\Psi_{n\boldsymbol{\lambda}}(t)\rangle = e^{i\gamma_n(t)}e^{-\frac{i}{\hbar}\int_0^t dt'\varepsilon_{n\boldsymbol{\lambda}(t')}}|n,\boldsymbol{\lambda}(t)\rangle. \tag{1.3}$$

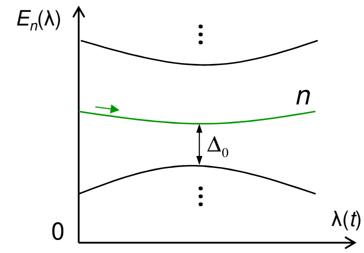

FIG. 1 If a Hamiltonian varies slowly with time, then an electron at state $|n,\boldsymbol{\lambda}\rangle$ would stay at the same level.

This extra phase had been deemed as removable with the help of the $\chi_n(\boldsymbol{\lambda})$ phase in Eq. (1.1) ever since the early days of quantum mechanics, until Berry showed the contrary in 1984 (Berry, 1984).

The phase γ_n is constrained by the time-dependent Schrödinger equation,

$$H|\Psi_{n\boldsymbol{\lambda}}(t)\rangle = i\hbar\frac{\partial}{\partial t}|\Psi_{n\boldsymbol{\lambda}(t)}\rangle. \tag{1.4}$$

Substitute Eq. (1.3) into Eq. (1.4), one has

$$\frac{d\gamma_n(t)}{dt} = i\langle n,\boldsymbol{\lambda}|\frac{\partial}{\partial t}|n,\boldsymbol{\lambda}\rangle \tag{1.5}$$

$$\to \quad \gamma_n(t) = i\int_0^t dt'\langle n,\boldsymbol{\lambda}|\frac{\partial}{\partial t'}|n,\boldsymbol{\lambda}\rangle. \tag{1.6}$$

For a cyclic change of the parameters,

$$\boldsymbol{\lambda}(0) \to \boldsymbol{\lambda}(T) = \boldsymbol{\lambda}(0), \tag{1.7}$$

one has,

$$\gamma_n(T) = i\oint_C d\boldsymbol{\lambda}\cdot\langle n,\boldsymbol{\lambda}|\frac{\partial}{\partial\boldsymbol{\lambda}}|n,\boldsymbol{\lambda}\rangle, \tag{1.8}$$

in which C is the loop traversed in the parameter space of $\boldsymbol{\lambda}$. $\gamma_n(T)$, or $\gamma_n(C)$, is the **Berry phase** acquired by $|\Psi_n\rangle$ after one cycle in energy level n. It depends only on the geometry of the path C, but not on the rate of $\dot{\boldsymbol{\lambda}}$, as long as it is slow enough so that inter-level transition can be neglected.

We will call the integrand in Eq. (1.8) the **Berry connection**,

$$\mathbf{A}_n(\boldsymbol{\lambda}) \equiv i\langle n,\boldsymbol{\lambda}|\frac{\partial}{\partial\boldsymbol{\lambda}}|n,\boldsymbol{\lambda}\rangle. \tag{1.9}$$

If one re-assigns a $\boldsymbol{\lambda}$-dependent phase to the snapshot state,

$$|n,\boldsymbol{\lambda}\rangle \to |n,\boldsymbol{\lambda}\rangle' = e^{i\chi(\boldsymbol{\lambda})}|n,\boldsymbol{\lambda}\rangle, \tag{1.10}$$

where $e^{i\chi(\boldsymbol{\lambda})}$ *is a single-valued function*, then

$$\mathbf{A}_n(\boldsymbol{\lambda}) \to \mathbf{A}'_n(\boldsymbol{\lambda}) = \mathbf{A}_n(\boldsymbol{\lambda}) - \frac{\partial\chi}{\partial\boldsymbol{\lambda}}. \tag{1.11}$$

This is similar to the **gauge transformation** of a vector potential in electromagnetism. Before Berry's discovery, people thought that by solving $\partial\chi(\boldsymbol{\lambda})/\partial\boldsymbol{\lambda} = \mathbf{A}_n(\boldsymbol{\lambda})$, $\mathbf{A}'_n(\boldsymbol{\lambda})$ can be set as zero and removed (Schiff, 1972). However, this is possible only if the loop integral for $\gamma_n(C)$ is zero. If not, then since $\gamma_n(C)$ (mod 2π) is gauge invariant,

$$\begin{aligned}\gamma'_n(C) &= \oint_C d\boldsymbol{\lambda}\cdot\mathbf{A}'_n(\boldsymbol{\lambda}) \\ &= \oint_C d\boldsymbol{\lambda}\cdot\mathbf{A}_n(\boldsymbol{\lambda}) - \chi(\boldsymbol{\lambda}(T)) + \chi(\boldsymbol{\lambda}(0)) \\ &= \gamma_n(C) + 2\pi\times\text{integer},\end{aligned} \tag{1.12}$$

it's impossible to remove $\mathbf{A}_n(\boldsymbol{\lambda})$ by gauge transformation.

If the parameter space is three-dimensional, then one can apply the **Stokes theorem** to write the Berry phase as a surface integral over the area S enclosed by the loop C,

$$\begin{aligned}\gamma_n(C) &= \int_S d^2\mathbf{a}\cdot\nabla_{\boldsymbol{\lambda}}\times\mathbf{A}_n & (1.13)\\ &= \int_S d^2\mathbf{a}\cdot\mathbf{F}_n, & (1.14)\end{aligned}$$

in which $\mathbf{F}_n \equiv \nabla_{\boldsymbol{\lambda}}\times\mathbf{A}_n$ is called the **Berry curvature**. In higher dimension, Stokes theorem remains valid, but needs be written in the language of **differential form** (see App. **??**).

For a small loop $\Box$,

$$\gamma_n(\Box) \simeq d^2\mathbf{a}\cdot\mathbf{F}_n, \tag{1.15}$$

where $d^2\mathbf{a} = d^2a\hat{\mathbf{n}}$. Hence,

$$\mathbf{F}_n\cdot\hat{\mathbf{n}} \simeq \frac{\gamma_n(\Box)}{d^2a}. \tag{1.16}$$

This becomes an equality when $d^2a \to 0$. That is, the Berry curvature at $\boldsymbol{\lambda}$ equals the ratio between the Berry phase for an infinitesimal loop around that point and the area of the loop.

Example: Consider a spin-1/2 electron in a magnetic field $\mathbf{B} = B\hat{n}$ (see Fig. 2), where $\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. The Hamiltonian is

$$H = -\boldsymbol{\mu}\cdot\mathbf{B} = \mu_B\boldsymbol{\sigma}\cdot\mathbf{B},\ \mu_B = \frac{e\hbar}{2m}. \tag{1.17}$$

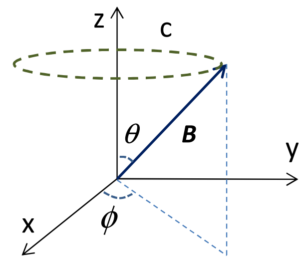

FIG. 2 A magnetic field sweeps slowly around the loop C.

The eigen-energies are $\varepsilon_\pm = \pm\mu_B B$, and the eigenstates are

$$|\hat{n},+\rangle = \begin{pmatrix}\cos\frac{\theta}{2}\\ e^{i\phi}\sin\frac{\theta}{2}\end{pmatrix},\ |\hat{n},-\rangle = \begin{pmatrix}-e^{-i\phi}\sin\frac{\theta}{2}\\ \cos\frac{\theta}{2}\end{pmatrix}. \tag{1.18}$$

Note that $e^{i\alpha_\pm\phi}|\hat{n},\pm\rangle$ are also eigenstates ($\alpha_\pm$ do not depend on angle), but they are not single-valued if $\alpha_\pm$ is not an integer. We emphasize that, *when calculating the Berry phase, the snapshot states in Eq. (1.8) need to be single-valued.* Even if one adopts only single-valued states, the choice of basis is still not unique. For example, $|\hat{n},\pm\rangle' = e^{\mp i\phi}|\hat{n},\pm\rangle$ are also single-valued. You can check that the ϕ's in $|\hat{n},\pm\rangle$ are ambiguous at $\theta=\pi$ (but not at $\theta=0$), while the ϕ's in $|\hat{n},\pm\rangle'$ are ambiguous at $\theta=0$ (but not at $\theta=\pi$).

The magnetic field $\mathbf{B}$ plays the role of the slowly varying parameters $\boldsymbol{\lambda}$. The Berry connection can be calculated from Eq. (1.9) with the gradient operator,

$$\frac{\partial}{\partial\mathbf{B}} = \frac{\partial}{\partial B}\hat{e}_r + \frac{1}{B}\frac{\partial}{\partial\theta}\hat{e}_\theta + \frac{1}{B\sin\theta}\frac{\partial}{\partial\phi}\hat{e}_\phi. \tag{1.19}$$

It is left as an exercise to show that

$$\begin{aligned}\mathbf{A}_+(\mathbf{B}) &= i\langle\hat{\mathbf{B}},+|\frac{\partial}{\partial\mathbf{B}}|\hat{\mathbf{B}},+\rangle & (1.20)\\ &= -\frac{1}{2B}\frac{1-\cos\theta}{\sin\theta}\hat{e}_\phi. & (1.21)\end{aligned}$$

Similarly,

$$\mathbf{A}_-(\mathbf{B}) = \frac{1}{2B}\frac{1-\cos\theta}{\sin\theta}\hat{e}_\phi. \tag{1.22}$$

Both $\mathbf{A}_\pm(\mathbf{B})$ are singular along $\theta=\pi$. These vector potentials are the same as that of a **magnetic monopole**, and the line of singularity corresponds to the **Dirac string** there.

The Berry curvature is,

$$\mathbf{F}_\pm(\mathbf{B}) = \nabla_{\mathbf{B}}\times\mathbf{A}_\pm(\mathbf{B}) = \mp\frac{1}{2}\frac{\hat{B}}{B^2}. \tag{1.23}$$

This is the same as the field of a magnetic monopole at the origin with a magnetic charge $\mp 1/2$.

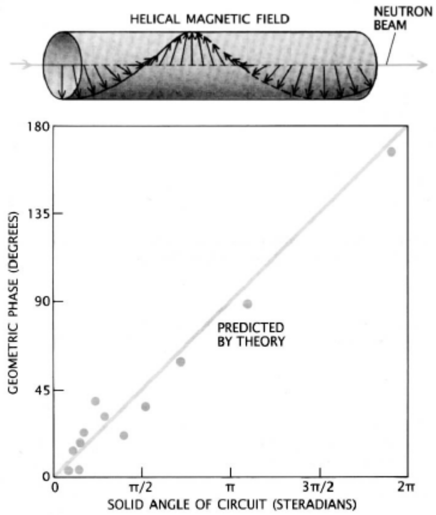

FIG. 3 Berry phase of an electron passing through a helical magnetic field (Bitter and Dubbers, 1987).

The Berry phase can be calculated using either the line integral of $\mathbf{A}_\pm$, or the surface integral of $\mathbf{F}_\pm$. For a loop in Fig. 2, the Berry phase is found to be,

$$\gamma_\pm(C) = \mp\frac{1}{2}\Omega(C), \tag{1.24}$$

where $\Omega(C) = 2\pi(1-\cos\theta)$ is the solid angle, as seen from the origin, extended by the loop C. If the loop is lying on the x-y-plane, then the Berry phase can only be $\mp\pi$. That is, the state changes sign after a cyclic evolution. The phase in Eq. (1.24) has been confirmed by passing neutrons through a tube with a helical magnetic field (Fig. 3).

Note that, given $|\hat{n},\pm\rangle' = e^{\mp i\phi}|\hat{n},\pm\rangle$, the Berry connections calculated from the two basis differ by a gradient,

$$\begin{aligned}\mathbf{A}'_\pm(\mathbf{B}) &= \mathbf{A}_\pm(\mathbf{B}) \pm \frac{\partial\phi}{\partial\mathbf{B}} &(1.25)\\ &= \mathbf{A}_\pm(\mathbf{B}) \pm \frac{1}{B\sin\theta}\hat{e}_\phi. &(1.26)\end{aligned}$$

Therefore,

$$\mathbf{A}'_\pm(\mathbf{B}) = \pm\frac{1}{2B}\frac{1+\cos\theta}{\sin\theta}\hat{e}_\phi. \tag{1.27}$$

Both $\mathbf{A}'_\pm(\mathbf{B})$ are singular along $\theta = 0$. They generate the same Berry curvatures as those in Eq. (1.23).

The integral of $\mathbf{F}_\pm$ over a closed surface enclosing the origin is quantized,

$$\frac{1}{2\pi}\int_{S_B^2} d^2\mathbf{a}\cdot\mathbf{F}_\pm(\mathbf{B}) = \mp 1. \tag{1.28}$$

This integer remains fixed no matter how the surface S_B^2 is deformed, as long as it is not torn up. This topological number is called the **first Chern number** in mathematics. It is also known as the **Berry index** (or the **topological charge**) of the degenerate point.

Finally, the analogy between the gauge structure of the Berry phase and that of the classical electromagnetism is summarized in Table I.

TABLE I Analogy between electromagnetism and anholonomy

Electromagnetism	Quantum anholonomy
vector potential $\mathbf{A}(\mathbf{r})$	Berry connection $\mathbf{A}(\boldsymbol{\lambda})$
magnetic field $\mathbf{B}(\mathbf{r})$	Berry curvature $\mathbf{F}(\boldsymbol{\lambda})$
magnetic monopole	degenerate point
magnetic charge	Berry index
magnetic flux $\Phi(C)$	Berry phase $\gamma(C)$

B. Geometric analogy

Berry phase is analogous to the anholonomy angle on a curved surface M. This is explained as follows. Suppose that at point p on M, there is an orthogonal frame $(\mathbf{n}, \tilde{\mathbf{e}}_1, \tilde{\mathbf{e}}_2)$, where $\mathbf{n}$ is the unit normal vector at p and $(\tilde{\mathbf{e}}_1, \tilde{\mathbf{e}}_2)$ is an orthonormal basis in the tangent plane, $\hat{\mathbf{n}} = \tilde{\mathbf{e}}_1 \times \tilde{\mathbf{e}}_2$ (see Fig. 4). As a rule of **parallel transport** (PT), we demand that, when moving along a curve C on M, the frame should *not* twist around $\mathbf{n}$ (see Berry's introductory article in Wilczek and Shapere, World Scientific). That is, if $\boldsymbol{\omega}$ is the angular velocity of the triad, then

$$\boldsymbol{\omega}\cdot\mathbf{n} = 0. \tag{1.29}$$

Also, one has $\dot{\tilde{\mathbf{e}}}_{\mathbf{1,2}} = \boldsymbol{\omega}\times\tilde{\mathbf{e}}_{\mathbf{1,2}}$. It follows that,

$$\begin{aligned}\boldsymbol{\omega}\cdot\mathbf{n} &= \boldsymbol{\omega}\cdot\tilde{\mathbf{e}}_1\times\tilde{\mathbf{e}}_2\\ &= \boldsymbol{\omega}\times\tilde{\mathbf{e}}_1\cdot\tilde{\mathbf{e}}_2 = \dot{\tilde{\mathbf{e}}}_1\cdot\tilde{\mathbf{e}}_2 = 0. &(1.30)\end{aligned}$$

Furthermore, since $\tilde{\mathbf{e}}_1\cdot\tilde{\mathbf{e}}_1 = \tilde{\mathbf{e}}_2\cdot\tilde{\mathbf{e}}_2 = 1$, one has $\dot{\tilde{\mathbf{e}}}_1\cdot\tilde{\mathbf{e}}_1 = \dot{\tilde{\mathbf{e}}}_2\cdot\tilde{\mathbf{e}}_2 = 0$.

If we introduce the following complex vector,

$$\psi = \frac{1}{\sqrt{2}}\left(\tilde{\mathbf{e}}_1 + i\tilde{\mathbf{e}}_2,\right). \tag{1.31}$$

then the PT condition can be rephrased as,

$$\mathrm{Im}\left(\psi^*\cdot\dot{\psi}\right) = 0, \text{ or } \psi^*\cdot\dot{\psi} = 0. \tag{1.32}$$

Note that the real part of $\psi^*\cdot\dot{\psi}$ is always zero.

Instead of this parallel-transported triad, we can erect a fixed triad $(\mathbf{n}, \mathbf{e}_1, \mathbf{e}_2)$ at each point on the surface. They

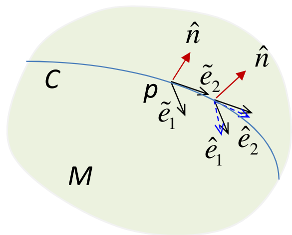

FIG. 4 A triad (solid lines) moves along a path C under the parallel transport condition. A fixed triad assigned to each point is indicated by dotted lines.

are required to vary smoothly, but are otherwise arbitrary. Introduce

$$\phi = \frac{1}{\sqrt{2}}\left(\mathbf{e}_1 + i\mathbf{e}_2\right). \tag{1.33}$$

Assuming these two frames differ by an angle $\alpha(\mathbf{r})$ around the $\mathbf{n}$-axis, then $\psi(\mathbf{r}) = \phi(\mathbf{r})e^{i\alpha(\mathbf{r})}$. It follows that

$$\psi^* \cdot d\psi = \phi^* \cdot d\phi + i d\alpha. \tag{1.34}$$

Because of the PT condition in Eq. (1.32), we have $d\alpha = i\phi^* \cdot d\phi$. Finally, the twist angle accumulated by the moving PT frame after completing a closed loop C is,

$$\alpha(C) = i\oint_C \phi^* \cdot \frac{d\phi}{d\mathbf{r}} \cdot d\mathbf{r}, \tag{1.35}$$

That is, the **anholonomy angle** $\alpha(C)$ can be calculated with the fixed, single-valued frames. This is analogous to the formula for Berry phase Eq. (1.8). In Table II, one can find more analogies between theories of anholonomy angle and Berry phase.

TABLE II Holonomies in geometry and quantum state

	geometry	quantum state
fixed basis	$\phi(x)$	$\vert\phi;\boldsymbol{\lambda}\rangle$
PT basis	$\psi(x)$	$\vert\psi;\boldsymbol{\lambda}\rangle$
PT condition	$\psi^*\cdot\dot{\psi}=0$	$\langle\psi\vert\dot{\psi}\rangle = 0$
holonomy	anholonomy angle	Berry phase
curvature	Gaussian curvature	Berry curvature
topological number	Euler characteristic	Chern number

C. Degenerate energy levels

One can extend the analysis above to degenerate energy levels (Wilczek and Zee, 1984). The wave function now has multiple components for a given energy level. As a result, the Berry connection and the Berry curvature become matrix-valued vectors (or vector-valued matrices). For simplicity, we consider an energy level $\varepsilon_{n\boldsymbol{\lambda}}$ with only two orthonormal, (globally) degenerate eigenstates, $|n, 1, \boldsymbol{\lambda}\rangle$ and $|n, 2, \boldsymbol{\lambda}\rangle$. Again $\boldsymbol{\lambda}$ are slowly varying parameters.

After time t, the states evolve to (compare with Eq. (1.3))

$$\begin{aligned}|\Psi_{n,1}(t)\rangle &= e^{-\frac{i}{\hbar}\int_0^t dt'\varepsilon_{n\boldsymbol{\lambda}(t')}} && (1.36)\\ &\quad\times\left(|n,1,\boldsymbol{\lambda}(t)\rangle\Gamma_{11}(t) + |n,2,\boldsymbol{\lambda}(t)\rangle\Gamma_{21}(t)\right),\\ |\Psi_{n,2}(t)\rangle &= e^{-\frac{i}{\hbar}\int_0^t dt'\varepsilon_{n\boldsymbol{\lambda}(t')}} && (1.37)\\ &\quad\times\left(|n,1,\boldsymbol{\lambda}(t)\rangle\Gamma_{12}(t) + |n,2,\boldsymbol{\lambda}(t)\rangle\Gamma_{22}(t)\right).\end{aligned}$$

Or, $(\alpha, \beta = 1, 2)$

$$|\Psi_{n\beta}(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t dt'\varepsilon_{n\boldsymbol{\lambda}(t')}}\sum_\alpha |n\alpha\boldsymbol{\lambda}(t)\rangle\Gamma_{\alpha\beta}(t). \tag{1.38}$$

We call the matrix $\Gamma_{\alpha\beta}$ a **Berry rotation matrix**. To be consistent with the orthonormal condition

$$\langle\Psi_{n\alpha}|\Psi_{n\beta}\rangle = \delta_{\alpha\beta}, \tag{1.39}$$

the Berry rotation matrix needs to be unitary,

$$\Gamma^\dagger\Gamma = \Gamma\Gamma^\dagger = 1. \tag{1.40}$$

Substitute the states into the Schrödinger equation,

$$H|\Psi_{n\beta}(t)\rangle = i\hbar\frac{\partial}{\partial t}|\Psi_{n\beta}(t)\rangle, \tag{1.41}$$

one will get,

$$\begin{aligned}\frac{d\Gamma_{\alpha\beta}}{dt} &= -\sum_\gamma\langle n\alpha\boldsymbol{\lambda}|\frac{\partial}{\partial t}|n\gamma\boldsymbol{\lambda}\rangle\Gamma_{\gamma\beta} && (1.42)\\ &= i\sum_\gamma\dot{\boldsymbol{\lambda}}(t)\cdot\mathbf{A}^{(n)}_{\alpha\gamma}(\boldsymbol{\lambda})\Gamma_{\gamma\beta}, && (1.43)\end{aligned}$$

where

$$\mathbf{A}^{(n)}_{\alpha\beta}(\boldsymbol{\lambda}) \equiv i\langle n\alpha\boldsymbol{\lambda}|\frac{\partial}{\partial\boldsymbol{\lambda}}|n\beta\boldsymbol{\lambda}\rangle. \tag{1.44}$$

The Berry connection now becomes a matrix-valued vector, $\vec{\mathsf{A}}^{(n)}$. To simplify the index, we focus only on one degenerate eigenenergy and suppress the index n from now on.

To solve for the $U(2)$ Berry rotation matrix $\Gamma(t)$, first consider an infinitesimal dt,

$$\begin{aligned}\Gamma(t+dt) &= \Gamma(t) + idt\dot{\boldsymbol{\lambda}}(t)\cdot\vec{\mathsf{A}}(t)\Gamma(t) && (1.45)\\ &\simeq e^{idt\dot{\boldsymbol{\lambda}}(t)\cdot\vec{\mathsf{A}}(t)}\Gamma(t) && (1.46)\end{aligned}$$

A full path can be divided into small steps, so that

$$\begin{aligned}\Gamma(t) &= \cdots e^{id\boldsymbol{\lambda}\cdot\vec{\mathsf{A}}(\boldsymbol{\lambda}_1)}e^{id\boldsymbol{\lambda}\cdot\vec{\mathsf{A}}(\boldsymbol{\lambda}_0)}\Gamma(0) && (1.47)\\ &\equiv Pe^{i\int_{\boldsymbol{\lambda}_0}^{\boldsymbol{\lambda}(t)}d\boldsymbol{\lambda}\cdot\vec{\mathsf{A}}(\boldsymbol{\lambda})},\ \Gamma(0)=1, && (1.48)\end{aligned}$$

in which P is a **path-ordering operator**. Because of the path-ordering, $\mathsf{\Gamma}(t)$ usually can only be computed numerically (see Sec. **??**).

Sometimes one can see non-Abelian Berry connections being calculated for energy levels that are not globally degenerate (or not degenerate at all). In such cases, the dynamical phase factor in Eq. (1.38) needs be changed to $e^{-\frac{i}{\hbar}\int_0^t dt' \varepsilon_{n\alpha\boldsymbol{\lambda}(t')}}$, and the right hand side of Eq. (1.43) is multiplied by $e^{-\frac{i}{\hbar}\int_0^t dt'(\varepsilon_{n\gamma\boldsymbol{\lambda}}-\varepsilon_{n\alpha\boldsymbol{\lambda}})}$. The Berry connection and Berry curvature can still be defined in the same manner, but the Berry rotation among these energy levels would be mixed with dynamical phase factors.

We now consider a gauge transformation,

$$|\alpha\boldsymbol{\lambda}\rangle' = \sum_\gamma |\gamma\boldsymbol{\lambda}\rangle U_{\gamma\alpha}(\boldsymbol{\lambda}). \tag{1.49}$$

Its dual is

$$\langle\alpha\boldsymbol{\lambda}|' = \sum_\gamma U^\dagger_{\alpha\gamma}(\boldsymbol{\lambda})\langle\gamma\boldsymbol{\lambda}|. \tag{1.50}$$

Therefore,

$$\begin{aligned} \mathbf{A}'_{\alpha\beta}(\boldsymbol{\lambda}) &= i\langle\alpha\boldsymbol{\lambda}|'\frac{\partial}{\partial\boldsymbol{\lambda}}|\beta\boldsymbol{\lambda}\rangle' & (1.51)\\ &= U^\dagger_{\alpha\gamma}\mathbf{A}_{\gamma\delta}U_{\delta\beta} + iU^\dagger_{\alpha\gamma}\frac{\partial}{\partial\boldsymbol{\lambda}}U_{\gamma\beta}. & (1.52)\end{aligned}$$

Or,

$$\mathsf{A}'_k = \mathsf{U}^\dagger\mathsf{A}_k\mathsf{U} + i\mathsf{U}^\dagger\frac{\partial}{\partial\lambda_k}\mathsf{U}. \tag{1.53}$$

The phase factor

$$\begin{aligned} e^{id\boldsymbol{\lambda}\cdot\vec{\mathsf{A}}'} &\simeq 1 + id\boldsymbol{\lambda}\cdot\vec{\mathsf{A}}' & (1.54)\\ &= 1 + id\boldsymbol{\lambda}\cdot\mathsf{U}^\dagger\vec{\mathsf{A}}\mathsf{U} - d\boldsymbol{\lambda}\cdot\mathsf{U}^\dagger\frac{\partial}{\partial\boldsymbol{\lambda}}\mathsf{U} & (1.55)\\ &\simeq \mathsf{U}^\dagger\left(1 + id\boldsymbol{\lambda}\cdot\vec{\mathsf{A}}\right)\left(\mathsf{U} - d\boldsymbol{\lambda}\cdot\frac{\partial}{\partial\boldsymbol{\lambda}}\mathsf{U}\right) & (1.56)\\ &\simeq \mathsf{U}^\dagger(\boldsymbol{\lambda})e^{id\boldsymbol{\lambda}\cdot\vec{\mathsf{A}}}\mathsf{U}(\boldsymbol{\lambda}-d\boldsymbol{\lambda}). & (1.57)\end{aligned}$$

Therefore, after a closed path,

$$\mathsf{\Gamma}'[C] = \mathsf{U}^\dagger(\boldsymbol{\lambda}_0)\mathsf{\Gamma}[C]\mathsf{U}(\boldsymbol{\lambda}_0). \tag{1.58}$$

That is, the non-Abelian Berry rotation is **gauge covariant**.

Berry curvature $\vec{\mathsf{F}}$ is defined as the Berry rotation $\mathsf{\Gamma}_\Box$ around an infinitesimal loop $\Box$ enclosing an area $d^2\mathbf{a}$, $\mathsf{\Gamma}_\Box = e^{i\vec{\mathsf{F}}_\Box\cdot d^2\mathbf{a}}$, or

$$i\vec{\mathsf{F}}_\Box\cdot\hat{\mathbf{n}} \equiv \frac{\mathsf{\Gamma}_\Box - 1}{d^2a}, \tag{1.59}$$

where $\hat{n}$ is the normal vector of the surface $d^2\mathbf{a}$.

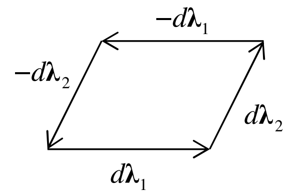

FIG. 5 A small loop in the parameter space of $\boldsymbol{\lambda}$.

The Berry rotation matrix is composed of 4 steps (see Fig. 5),

$$\begin{aligned} &\mathsf{\Gamma}_\Box(\boldsymbol{\lambda}) & (1.60)\\ &= \mathsf{\Gamma}(\boldsymbol{\lambda},\boldsymbol{\lambda}+d\boldsymbol{\lambda}_2)\mathsf{\Gamma}(\boldsymbol{\lambda}+d\boldsymbol{\lambda}_2,\boldsymbol{\lambda}+d\boldsymbol{\lambda}_1+d\boldsymbol{\lambda}_2)\\ &\times\ \mathsf{\Gamma}(\boldsymbol{\lambda}+d\boldsymbol{\lambda}_1+d\boldsymbol{\lambda}_2,\boldsymbol{\lambda}+d\boldsymbol{\lambda}_1)\mathsf{\Gamma}(\boldsymbol{\lambda}+d\boldsymbol{\lambda}_1,\boldsymbol{\lambda}).\end{aligned}$$

Using the approximation,

$$e^{\epsilon\mathsf{A}}e^{\epsilon\mathsf{B}} = e^{\epsilon(\mathsf{A}+\mathsf{B})+\frac{\epsilon^2}{2}[\mathsf{A},\mathsf{B}]} + O(\epsilon^3), \tag{1.61}$$

one has

$$\begin{aligned} &\mathsf{\Gamma}(\boldsymbol{\lambda}+d\boldsymbol{\lambda}_1+d\boldsymbol{\lambda}_2,\boldsymbol{\lambda}+d\boldsymbol{\lambda}_1)\mathsf{\Gamma}(\boldsymbol{\lambda}+d\boldsymbol{\lambda}_1,\boldsymbol{\lambda})\\ &= e^{i\mathsf{A}_k(\boldsymbol{\lambda}+d\boldsymbol{\lambda}_1)d\lambda_{2k}}e^{i\mathsf{A}_\ell(\boldsymbol{\lambda})d\lambda_{1\ell}} & (1.62)\\ &\simeq e^{i(\mathsf{A}_k d\lambda_{2k}+\mathsf{A}_\ell d\lambda_{1\ell}+\partial_\ell\mathsf{A}_k d\lambda_{2k}d\lambda_{1\ell})-\frac{1}{2}[\mathsf{A}_k,\mathsf{A}_\ell]d\lambda_{2k}d\lambda_{1\ell}}. & (1.63)\end{aligned}$$

For the next two steps, it is convenient to adopt instead (see p. 239 of Cheng and Li, 1988),

$$\begin{aligned} &\mathsf{\Gamma}^{-1}(\boldsymbol{\lambda}+d\boldsymbol{\lambda}_2,\boldsymbol{\lambda})\mathsf{\Gamma}^{-1}(\boldsymbol{\lambda}+d\boldsymbol{\lambda}_1+d\boldsymbol{\lambda}_2,\boldsymbol{\lambda}+d\boldsymbol{\lambda}_2)\\ &= e^{-i\mathsf{A}_k(\boldsymbol{\lambda})d\lambda_{2k}}e^{-i\mathsf{A}_\ell(\boldsymbol{\lambda}+d\boldsymbol{\lambda}_2)d\lambda_{1\ell}} & (1.64)\\ &\simeq e^{-i(\mathsf{A}_k d\lambda_{2k}+\mathsf{A}_\ell d\lambda_{1\ell}+\partial_k\mathsf{A}_\ell d\lambda_{2k}d\lambda_{1\ell})-\frac{1}{2}[\mathsf{A}_k,\mathsf{A}_\ell]d\lambda_{2k}d\lambda_{1\ell}}. & (1.65)\end{aligned}$$

Therefore,

$$\begin{aligned} \mathsf{\Gamma}_\Box &= e^{-i(\partial_k\mathsf{A}_\ell-\partial_\ell\mathsf{A}_k-i[\mathsf{A}_k,\mathsf{A}_\ell])d\lambda_{2k}d\lambda_{1\ell}} & (1.66)\\ &= e^{i\mathsf{F}_{k\ell}d\lambda_{1k}d\lambda_{2\ell}}, & (1.67)\end{aligned}$$

with the Berry curvature matrix,

$$\mathsf{F}_{k\ell} = \partial_k\mathsf{A}_\ell - \partial_\ell\mathsf{A}_k - i[\mathsf{A}_k,\mathsf{A}_\ell]. \tag{1.68}$$

Under a gauge transformation,

$$\begin{aligned} \mathsf{F}_{k\ell}\to\mathsf{F}'_{k\ell} &= \partial_k\mathsf{A}'_\ell - \partial_\ell\mathsf{A}'_k - i[\mathsf{A}'_k,\mathsf{A}'_\ell] & (1.69)\\ &= \mathsf{U}^\dagger\mathsf{F}_{k\ell}\mathsf{U}. & (1.70)\end{aligned}$$

That is, the non-Abelian Berry curvature is gauge covariant (similarly for $\vec{\mathsf{F}}$).

Note that $\mathsf{F}_{k\ell}$ is antisymmetric in k,ℓ, and

$$\mathsf{F}_{k\ell}d\lambda_{1k}d\lambda_{2\ell} = \frac{1}{2}\epsilon_{cab}\mathsf{F}_{ab}\ \epsilon_{ck\ell}d\lambda_{1k}d\lambda_{2\ell}, \tag{1.71}$$

in which $\frac{1}{2}\epsilon_{cab}\mathsf{F}_{ab} = \mathsf{F}_c$ is the vector equivalent of the antisymmetric matrix, and $\epsilon_{ck\ell}d\lambda_{1k}d\lambda_{2\ell} = (d^2\mathbf{a})_c$. Therefore,

$$\mathsf{F}_{k\ell}d\lambda_{1k}d\lambda_{2\ell} = \vec{\mathsf{F}}\cdot d^2\mathbf{a}, \tag{1.72}$$

When written in the vectorial form, the Berry curvature is (cf. Eq. (1.68)),

$$\vec{\mathsf{F}} = \nabla_{\boldsymbol{\lambda}} \times \vec{\mathsf{A}} - i\vec{\mathsf{A}} \times \vec{\mathsf{A}}. \tag{1.73}$$

Exercise

1. Replace the single-valued snapshot states $|n, \boldsymbol{\lambda}\rangle$ with $|n, \boldsymbol{\lambda}\rangle' = e^{i\gamma_n(t)}|n, \boldsymbol{\lambda}\rangle$, which are not necessarily single-valued. Show that

$$'\langle n, \boldsymbol{\lambda}| \frac{\partial}{\partial t} |n, \boldsymbol{\lambda}\rangle' = 0. \tag{1.74}$$

A state that evolves under such a restriction is said to be parallel transported. A state that moves under such a **parallel transport condition** acquires a Berry phase $\gamma_n(C)$ after a cycle C.

2. For a spin-1/2 electron in a magnetic field $\mathbf{B} = B\hat{n}, \hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, the eigenstates are,

$$|\hat{n}, +\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}, \ |\hat{n}, -\rangle = \begin{pmatrix} -e^{-i\phi}\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix}.$$

(a) Show that the Berry connections are,

$$\mathbf{A}_\pm(\mathbf{B}) = \mp\frac{1}{2B}\frac{1-\cos\theta}{\sin\theta}\hat{e}_\phi.$$

(b) Show that the Berry curvatures are,

$$\mathbf{F}_\pm(\mathbf{B}) = \mp\frac{1}{2}\frac{\hat{B}}{B^2}.$$

3. An electron moving in a magnetic field $\mathbf{B}(\mathbf{r}, t)$ has the Hamiltonian,

$$H = \frac{p^2}{2m} + \mathbf{B}(\mathbf{r}, t)\cdot\boldsymbol{\sigma}. \tag{1.75}$$

Suppose the eigenstates of the Zeeman term are $|n, \mathbf{B}(\mathbf{r})\rangle$,

$$\mathbf{B}(\mathbf{r}, t)\cdot\boldsymbol{\sigma}|n, \mathbf{B}(\mathbf{r}, t)\rangle = \varepsilon_n|n, \mathbf{B}(\mathbf{r}, t)\rangle, \tag{1.76}$$

expand the wave function of the moving electron as,

$$|\Psi\rangle = \sum_{n=\pm}\psi_n(\mathbf{r}, t)|n, \mathbf{B}\rangle. \tag{1.77}$$

From the Schrödinger equation, $H|\Psi\rangle = i\hbar\partial|\Psi\rangle/\partial t$, show that,

$$\left[\frac{1}{2m}\left(\mathbf{p} - \hbar\mathbf{A}_n\right)^2 + \hbar V_n + \varepsilon_n\right]\psi_n = i\hbar\frac{\partial\psi_n}{\partial t}, \tag{1.78}$$

in which

$$\begin{aligned} \mathbf{A}_n(\mathbf{r}, t) &= +i\langle n, \mathbf{B}|\frac{\partial}{\partial\mathbf{r}}|n, \mathbf{B}\rangle, && (1.79) \\ V_n(\mathbf{r}, t) &= -i\langle n, \mathbf{B}|\frac{\partial}{\partial t}|n, \mathbf{B}\rangle. && (1.80) \end{aligned}$$

The off-diagonal coupling between $|+\rangle$ and $|-\rangle$ has been ignored (this is all right for a smooth magnetic field).

That is, the effective Hamiltonian for the particle motion acquires a Berry potential $\mathbf{A}_n$ and a scalar potential V_n. Such potentials would result in forces (proportional to Berry curvatures) that act on the electron.

For example, the $\mathbf{B}$ field here can be an effective magnetic field from a spin texture, such as a **magnetic skyrmion** (see Nagaosa and Tokura, 2013). An electron moving near a magnetic skyrmion would feel such forces.

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