Lecture notes on topological insulators

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CONTENTS

I. BERRY CURVATURE OF BLOCH STATES

A. Basics of Bloch state

For a perfect crystal with discrete translation symmetry, the Hamiltonian is

$$H = \frac{p^2}{2m} + V_L(\mathbf{r}),\ \text{with } V_L(\mathbf{r}+\mathbf{R}) = V_L(\mathbf{r}), \tag{1.1}$$

in which $V_L(\mathbf{r})$ is the potential of the atomic lattice, and $\mathbf{R}$ is a **lattice translation vector**. Define a **lattice translation operator** $T_\mathbf{R}$ that acts on electronic states as follows,

$$T_\mathbf{R}\psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{R}). \tag{1.2}$$

It can be shown that, because H has the translation symmetry,

$$T_\mathbf{R}H(\mathbf{r})\psi(\mathbf{r}) = H(\mathbf{r})T_\mathbf{R}\psi(\mathbf{r}). \tag{1.3}$$

That is, $[T_\mathbf{R}, H] = 0$.

Because $T_\mathbf{R}$ commutes with $H(\mathbf{r})$, one can find their simultaneous eigenstates,

$$\begin{aligned} H\psi &= \varepsilon\psi, & (1.4)\\ T_\mathbf{R}\psi &= c_\mathbf{R}\psi, & (1.5)\end{aligned}$$

where ε and $c_\mathbf{R}$ are eigenvalues of H and $T_\mathbf{R}$, and $|c_\mathbf{R}| = 1$. Furthermore, successive translations satisfy

$$T_\mathbf{R}T_{\mathbf{R}'} = T_{\mathbf{R}'}T_\mathbf{R} = T_{\mathbf{R}+\mathbf{R}'}. \tag{1.6}$$

This leads to

$$c_\mathbf{R}c_{\mathbf{R}'} = c_{\mathbf{R}'}c_\mathbf{R} = c_{\mathbf{R}+\mathbf{R}'}. \tag{1.7}$$

To satisfy these equations, $c_\mathbf{R}$ needs to be an exponential, $c_\mathbf{R} = e^{i\mathbf{k}\cdot\mathbf{R}}$. Therefore,

$$\begin{aligned} H\psi_{\varepsilon\mathbf{k}} &= \varepsilon\psi_{\varepsilon\mathbf{k}}, & (1.8)\\ T_\mathbf{R}\psi_{\varepsilon\mathbf{k}} &= e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{\varepsilon\mathbf{k}}. & (1.9)\end{aligned}$$

The simultaneous eigenstate of H and $T_\mathbf{R}$ is called **Bloch state**.

If one writes the Bloch state in the following form,

$$\psi_{\varepsilon\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\varepsilon\mathbf{k}}(\mathbf{r}), \tag{1.10}$$

then Eq. (1.9) gives

$$u_{\varepsilon\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{\varepsilon\mathbf{k}}(\mathbf{r}). \tag{1.11}$$

That is, a Bloch state is a plane wave times a **cell-periodic function** $u_{\varepsilon\mathbf{k}}(\mathbf{r})$. The latter contains, *in one unit cell*, all information of the Bloch state $\psi_{\varepsilon\mathbf{k}}$.

The Schrödinger equation for $u_{\varepsilon\mathbf{k}}$ is,

$$\tilde{H}_\mathbf{k}(\mathbf{r})u_{\varepsilon\mathbf{k}} = \varepsilon u_{\varepsilon\mathbf{k}}, \tag{1.12}$$

in which

$$\begin{aligned} \tilde{H}_\mathbf{k}(\mathbf{r}) &\equiv e^{-i\mathbf{k}\cdot\mathbf{r}}H(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} & (1.13)\\ &= \frac{1}{2m}(\mathbf{p}+\hbar\mathbf{k})^2 + V_L(\mathbf{r}). & (1.14)\end{aligned}$$

Since $u_{\varepsilon\mathbf{k}}$ can be restricted to one unit cell (with periodic boundary condition), we expect it to have discrete energy eigenvalues ε_n $(n \in Z^+)$ for each $\mathbf{k}$, and write

$$\tilde{H}_\mathbf{k}(\mathbf{r})u_{n\mathbf{k}} = \varepsilon_{n\mathbf{k}}u_{n\mathbf{k}}. \tag{1.15}$$

The quantum numbers n and $\mathbf{k}$ are called **band index** and **Bloch momentum**, and $\varepsilon_{n\mathbf{k}}$ are the energy dispersions of Bloch bands.

The Bloch state $\psi_{n\mathbf{k}}$ translates under $\mathbf{R}$ as (see Eq. (1.9)),

$$\psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r}). \tag{1.16}$$

If one shifts the momentum $\mathbf{k}$ by a **reciprocal lattice vector G**, then since $e^{i\mathbf{G}\cdot\mathbf{R}} = 1$ (for any $\mathbf{R}$),

$$\psi_{n\mathbf{k}+\mathbf{G}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}+\mathbf{G}}(\mathbf{r}). \tag{1.17}$$

Since the two Bloch states $\psi_{n\mathbf{k}}$ and $\psi_{n\mathbf{k}+\mathbf{G}}$ satisfy the same Schrödinger equation (with $\varepsilon_{n\mathbf{k}} = \varepsilon_{n\mathbf{k}+\mathbf{G}}$) and the same boundary condition (Eqs. (1.16)and (1.17)), they can differ (for non-degenerate states) at most by a phase factor $\phi(\mathbf{k})$. For convenience, one can choose the **periodic gauge** with $\phi(\mathbf{k}) = 0$, $\psi_{n\mathbf{k}+\mathbf{G}} = \psi_{n\mathbf{k}}$. Note that for a quantum phase with non-trivial topology (such as the quantum Hall state), one can no longer set $\phi(\mathbf{k}) = 0$ for *all* $\mathbf{k}$. This is called **topological obstruction** (see Chap. I). In any case, $\psi_{n\mathbf{k}}$ (or $u_{n\mathbf{k}}$) in the first Brillouin zone should contain enough information of the electronic state.

The Bloch momentum plays the role of the slowly varying parameter, so the Berry connection for band-n is

$$\mathbf{A}_n(\mathbf{k}) = i\langle u_{n\mathbf{k}}|\frac{\partial}{\partial\mathbf{k}}|u_{n\mathbf{k}}\rangle. \tag{1.18}$$

The Berry curvature is

$$\begin{aligned}\mathbf{F}_n(\mathbf{k}) &= \nabla_{\mathbf{k}} \times \mathbf{A}_n(\mathbf{k}) & (1.19)\\ &= i\langle\frac{\partial u_{n\mathbf{k}}}{\partial\mathbf{k}}| \times |\frac{\partial u_{n\mathbf{k}}}{\partial\mathbf{k}}\rangle. & (1.20)\end{aligned}$$

Under time reversal, the Bloch states transform as

$$\psi_{n\mathbf{k}} \to \Theta\psi_{n\mathbf{k}} = \psi^*_{n\mathbf{k}}. \tag{1.21}$$

The transformed cell-periodic functions satisfy

$$\left[\frac{(\mathbf{p}-\hbar\mathbf{k})^2}{2m} + V_L(\mathbf{r})\right] u^*_{n\mathbf{k}} = \varepsilon_{n\mathbf{k}} u^*_{n\mathbf{k}}. \tag{1.22}$$

If the system has time-reversal symmetry, then the Schrödinger equation has to be invariant under the transformation. This shows that

$$u_{n\mathbf{k}}(\mathbf{r}) \to \Theta u_{n\mathbf{k}}(\mathbf{r}) = u^*_{n-\mathbf{k}}(\mathbf{r}). \tag{1.23}$$

Therefore,

$$\begin{aligned}\mathbf{A}_n(\mathbf{k}) &\to i\langle u^*_{n-\mathbf{k}}|\frac{\partial}{\partial\mathbf{k}}|u^*_{n-\mathbf{k}}\rangle & (1.24)\\ &= -i\langle u_{n-\mathbf{k}}|\frac{\partial}{\partial\mathbf{k}}|u_{n-\mathbf{k}}\rangle = \mathbf{A}_n(-\mathbf{k}) & \\ \mathbf{F}_n(\mathbf{k}) &\to \nabla_{\mathbf{k}} \times \mathbf{A}_n(-\mathbf{k}) = -\mathbf{F}_n(-\mathbf{k}) & (1.25)\end{aligned}$$

Similarly, if the crystal has space-inversion symmetry, then under the transformation,

$$u_{n\mathbf{k}}(\mathbf{r}) \to u_{n-\mathbf{k}}(-\mathbf{r}). \tag{1.26}$$

It follows that

$$\begin{aligned}\mathbf{A}_n(\mathbf{k}) &\to i\langle u_{n-\mathbf{k}}|\frac{\partial}{\partial\mathbf{k}}|u_{n-\mathbf{k}}\rangle = -\mathbf{A}_n(-\mathbf{k}), & (1.27)\\ \mathbf{F}_n(\mathbf{k}) &\to \nabla_{\mathbf{k}} \times [-\mathbf{A}_n(-\mathbf{k})] = \mathbf{F}_n(-\mathbf{k}). & (1.28)\end{aligned}$$

Therefore, if a crystal has both symmetries (and if the energy level is not degenerate), then $\mathbf{F}_n(\mathbf{k}) = 0$ for all $\mathbf{k}$, and one does not need to worry about the Berry curvature. Note: *One-dimensional* system is an exception. There can be Berry phase even if the system has both symmetries (more in next Lect).

B. Electric response of Bloch state

If the Berry curvature does exist, then it could influence the electron transport. For example, under an electric field $\mathbf{E}$, the velocity of an electron in Bloch state $\psi_{n\mathbf{k}}$ is

$$\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial\varepsilon_{n\mathbf{k}}}{\partial\mathbf{k}} + \frac{e}{\hbar}\mathbf{E} \times \mathbf{F}_n(\mathbf{k}). \tag{1.29}$$

This expression is valid if the electric field is weak so that inter-band transitions can be ignored. That is, an electron stays in the same energy band. This is called **one-band approximation**, which is the same as the adiabatic approximation.

Pf: Choose a *time-dependent* gauge for the electric field, $\mathbf{E} = -\partial\mathbf{A}/\partial t$, $\mathbf{A} = -\mathbf{E}t$, then the Hamiltonian becomes,

$$\tilde{H}^{\mathbf{E}}_{\mathbf{k}_0} = \frac{(\mathbf{p}+\hbar\mathbf{k}_0 - e\mathbf{E}t)^2}{2m} + V_L(\mathbf{r}) = \tilde{H}_{\mathbf{k}(t)}, \tag{1.30}$$

where $\mathbf{k}(t) = \mathbf{k}_0 - e\mathbf{E}t/\hbar$. For a weak field, to the zeroth order adiabatic approximation, one only needs to replace $|u_{n\mathbf{k}}\rangle$ with $|u_{n\mathbf{k}(t)}\rangle$, and

$$\tilde{H}_{\mathbf{k}(t)}|u_{n\mathbf{k}(t)}\rangle = \varepsilon_{n\mathbf{k}(t)}|u_{n\mathbf{k}(t)}\rangle. \tag{1.31}$$

To the first-order (see Prob. 1),

$$|u^{(1)}_{n\mathbf{k}}\rangle = |u_{n\mathbf{k}}\rangle - i\hbar\sum_{n'(\neq n)}\frac{|u_{n'\mathbf{k}}\rangle\langle u_{n'\mathbf{k}}|\frac{\partial}{\partial t}|u_{n\mathbf{k}}\rangle}{\varepsilon_{n\mathbf{k}} - \varepsilon_{n'\mathbf{k}}}, \tag{1.32}$$

in which all of the $\mathbf{k}$'s are $\mathbf{k}(t)$'s. Note that since $\langle u_{n\mathbf{k}}|u^{(1)}_{n\mathbf{k}}\rangle = 1$, an electron stays at the same energy level to this order.

To the first order, the velocity

$$\begin{aligned}\mathbf{v}_n(\mathbf{k}) &= \langle\psi^{(1)}_{n\mathbf{k}}|\frac{\mathbf{p}}{m}|\psi^{(1)}_{n\mathbf{k}}\rangle & (1.33)\\ &= \langle u^{(1)}_{n\mathbf{k}}|\frac{\mathbf{p}+\hbar\mathbf{k}}{m}|u^{(1)}_{n\mathbf{k}}\rangle & (1.34)\\ &= \langle u^{(1)}_{n\mathbf{k}}|\frac{\partial\tilde{H}_{\mathbf{k}}}{\hbar\partial\mathbf{k}}|u^{(1)}_{n\mathbf{k}}\rangle. & (1.35)\end{aligned}$$

Substitute Eqs. (1.32) into (1.35), one will get

$$\begin{aligned}\mathbf{v}_n(\mathbf{k}) &= \langle u_{n\mathbf{k}}|\frac{\partial\tilde{H}_{\mathbf{k}}}{\hbar\partial\mathbf{k}}|u_{n\mathbf{k}}\rangle & (1.36)\\ &- i\sum_{n'(\neq n)}\left(\frac{\langle u_{n\mathbf{k}}|\frac{\partial\tilde{H}_{\mathbf{k}}}{\partial\mathbf{k}}|u_{n'\mathbf{k}}\rangle\langle u_{n'\mathbf{k}}|\frac{\partial u_{n\mathbf{k}}}{\partial t}\rangle}{\varepsilon_{n\mathbf{k}} - \varepsilon_{n'\mathbf{k}}} - c.c.\right).\end{aligned}$$

Before proceeding further, some identities are required. First, starting from

$$\langle u_{n\mathbf{k}}|u_{n'\mathbf{k}}\rangle = \delta_{nn'}, \tag{1.37}$$

take the derivative $\partial/\partial\mathbf{k}$ to get

$$\langle\frac{\partial u_{n\mathbf{k}}}{\partial\mathbf{k}}|u_{n'\mathbf{k}}\rangle = -\langle u_{n\mathbf{k}}|\frac{\partial u_{n'\mathbf{k}}}{\partial\mathbf{k}}\rangle. \tag{1.38}$$

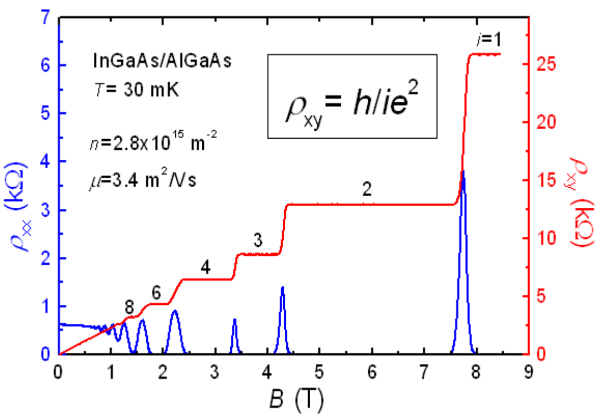

FIG. 1 The dependence of Hall resistivity (in red) on magnetic field shows quantized plateaus at $\rho_{xy} = h/(ie^2)$, where i is an integer. The resistivity at plateaus can be determined with very high precision. Thus, in 1990, h/e^2 is *defined* to be 25.812807 kΩ.

Second, from the equation,

$$\langle u_{n\mathbf{k}}|\tilde{H}_{\mathbf{k}}|u_{n'\mathbf{k}}\rangle = \varepsilon_{n\mathbf{k}}\delta_{nn'}, \tag{1.39}$$

take the derivative $\partial/\partial\mathbf{k}$ to get

$$\begin{aligned}\langle u_{n\mathbf{k}}|\frac{\partial \tilde{H}_{\mathbf{k}}}{\partial\mathbf{k}}|u_{n'\mathbf{k}}\rangle &= (\varepsilon_{n\mathbf{k}} - \varepsilon_{n'\mathbf{k}})\,\langle\frac{\partial u_{n\mathbf{k}}}{\partial\mathbf{k}}|u_{n'\mathbf{k}}\rangle \\ &+ \frac{\partial\varepsilon_{n\mathbf{k}}}{\hbar\partial\mathbf{k}}\delta_{nn'}. \end{aligned}\tag{1.40}$$

With the help of Eqs. (1.38) and (1.40), the velocity can be written as,

$$\begin{aligned}&\mathbf{v}_n(\mathbf{k}) \\ =\;& \frac{\partial\varepsilon_{n\mathbf{k}}}{\hbar\partial\mathbf{k}} - i\left(\left\langle\frac{\partial u_{n\mathbf{k}}}{\partial\mathbf{k}}|\frac{\partial u_{n\mathbf{k}}}{\partial t}\right\rangle - \left\langle\frac{\partial u_{n\mathbf{k}}}{\partial t}|\frac{\partial u_{n\mathbf{k}}}{\partial\mathbf{k}}\right\rangle\right) &(1.41)\\ =\;& \frac{\partial\varepsilon_{n\mathbf{k}}}{\hbar\partial\mathbf{k}} - \dot{\mathbf{k}}\times\mathbf{F}_n. &(1.42)\end{aligned}$$

Since $\dot{\mathbf{k}} = -(e/\hbar)\mathbf{E}$, the second term is $(e/\hbar)\mathbf{E}\times\mathbf{F}_n$. QED.

The velocity that depends on the Berry curvature is *perpendicular* to the direction of the applied **E** field. It first appeared in the study of **anomalous Hall effect** in Karplus and Luttinger, 1954, although not in the language of Berry curvature. This velocity proportional to the Berry curvature is sometimes called **anomalous velocity**.

Under the one-band approximation, Eq. (1.42) remains valid in the presence of a magnetic field **B**, but its derivation is not as easy. The **semiclassical equations of motion** for an electron in band-n are,

$$\begin{cases}\dot{\mathbf{r}} = \frac{\partial\varepsilon^m_{n\mathbf{k}}}{\hbar\partial\mathbf{k}} - \dot{\mathbf{k}}\times\mathbf{F}_n, \\ \hbar\dot{\mathbf{k}} = -e\mathbf{E} - e\dot{\mathbf{r}}\times\mathbf{B}.\end{cases}\tag{1.43}$$

in which $\varepsilon^m_{n\mathbf{k}} = \varepsilon_{n\mathbf{k}} - \mathbf{m}_n(\mathbf{k})\cdot\mathbf{B}$ is the energy shifted by magnetic moment $\mathbf{m}_n(\mathbf{k})$ (Chang and Niu, 1996; Sundaram and Niu, 1999).

C. Quantum Hall effect

The anomalous velocity plays a key role in the theory of **Quantum Hall effect** (QHE) and **Quantum anomalous Hall effect** (QAHE). We discuss the former in this section, and the latter in a later Lecture. For an early history regarding the discovery of the classical Hall effect, see Leadstone, 1979.

Consider a 2D electron gas (2DEG) lying on the x-y plane, such as the 2DEG in MOSFET, semiconductor heterojunction, graphene, or other 2D materials. Under a strong magnetic field $B\hat{z}$, the Landau levels of the 2DEG usually have non-zero Chern numbers. With a Berry curvature F_z along z-direction, the current density along x-direction is,

$$\begin{aligned}J_x &= -\frac{e}{L^2}\sum_{n\mathbf{k}} f(\varepsilon_{n\mathbf{k}})v_{nx}(\mathbf{k}) &(1.44)\\ &= -\frac{e}{L^2}\sum_{n\mathbf{k}} f(\varepsilon_{n\mathbf{k}})\frac{\partial\varepsilon_{n\mathbf{k}}}{\hbar\partial k_x} &(1.45)\\ &- \frac{e^2}{\hbar}\sum_n\frac{1}{L^2}\sum_{\mathbf{k}} f(\varepsilon_{n\mathbf{k}})F_{nz}(\mathbf{k})E_y, &(1.46)\end{aligned}$$

where L^2 is the area of the 2DEG, and $f(\varepsilon_{n\mathbf{k}})$ is the Fermi-Dirac distribution function. The first term is the current density in equilibrium, which is obviously zero. The second term contributes to the Hall current.

Note that the magnetic field **B** in Eq. (1.43) does not appear in this calculation, since it is responsible for the generation of the Landau levels and has been accounted for.

At temperature $T = 0$, if N energy bands (Landau sub-bands, to be precise) are filled, then the **Hall conductivity** is,

$$\begin{aligned}\sigma_{xy} &= -\frac{e^2}{\hbar}\frac{1}{L^2}\sum_{n,\mathbf{k}} F_{nz}(\mathbf{k}) &(1.47)\\ &= -\frac{e^2}{h}\sum_{n=1}^{N}\left(\frac{1}{2\pi}\int_{BZ} d^2k F_{nz}(\mathbf{k})\right). &(1.48)\end{aligned}$$

The integral over the Brillouin zone inside the parenthesis is an integer (see Eq. (1.61)). It is a topological quantity (Thouless *et al.*, 1982) called the **first Chern number**,

$$C_1^{(n)} = \frac{1}{2\pi}\int_{BZ} d^2k F_{nz}(\mathbf{k}) \in Z. \tag{1.49}$$

Therefore, an insulator with N filled bands would have a quantized quantum Hall conductance $(\sum_{n=1}^N C_1^{(n)})e^2/h$ (Fig. 1), independent of the details of energy bands.

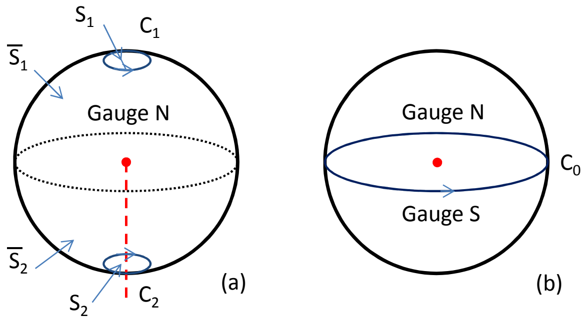

FIG. 2 (a) Gauge-N has a string of singularity along $-z$-axis. (b) An atlas with two patches of gauge is singularity-free.

The quantum Hall effect is first discovered accidentally by Klitzing *et al.*, 1980 in 2DEG. It has henceforth been observed in two-dimensional materials such as graphene and WSe_2 (a Transition Metal Dichalcogenide), among others. In order to have the QHE or the QAHE, the system has to be two-dimensional, since the topological Chern number is defined only in *even* dimensions. Also, the time-reversal symmetry needs to be broken, either by magnetic field or by magnetization. Finally, there has to be energy bands with nonzero Chern numbers that are completely filled. In practice, we usually need a low-temperature environment to avoid thermal excitations across the energy gap, and a high magnetic field to enlarge the energy gap (again to avoid thermal excitations). If the gap energy is much larger than thermal energy, then it is possible to have a room-temperature QHE (Novoselov *et al.*, 2007).

D. Gauge choice of Bloch state

Before discussing the gauge choice of Bloch state, let us look back at a simpler example: the spin-1/2 system in **??**. Recall that there are two types of basis:
$|\hat{n},\pm\rangle$ in Eq. (**??**), which have the ϕ-ambiguity at $\theta=\pi$;
$|\hat{n},\pm\rangle'=e^{\mp i\phi}|\hat{n},\pm\rangle$, which have the ϕ-ambiguity at $\theta=0$.

The Berry connection of the first basis is

$$\mathbf{A}^N_\pm(\mathbf{B})=\mp\frac{1}{2B}\frac{1-\cos\theta}{\sin\theta}\hat{e}_\phi. \tag{1.50}$$

It is singular along the axis of $\theta=\pi$ (see Fig. 2(a)), because of the ϕ-ambiguity mentioned above. However, the Berry curvature $\mathbf{F}_\pm=\mp\frac{1}{2}\frac{\hat{B}}{B^2}$ is well behaved along $\theta=\pi$.

On the other band, the Berry connection for the second basis is

$$\mathbf{A}^S_\pm(\mathbf{B})=\pm\frac{1}{2B}\frac{1+\cos\theta}{\sin\theta}\hat{e}_\phi. \tag{1.51}$$

It is singular along the axis of $\theta=0$. Both $\mathbf{A}^N_\pm$ and $\mathbf{A}^S_\pm$ have the same Berry curvature $\mathbf{F}_\pm$.

In Fig. 2(a), we see a loop C_1 near the north pole, and a loop C_2 near the south pole. The area inside C_1 is designated as S_1; the area outside is $\bar{S}_1$. Similarly the area inside C_2 is S_2, outside is $\bar{S}_2$. It is not difficult to see that,

$$\oint_{C_2} d\boldsymbol{\ell}\cdot\mathbf{A}^N_\pm=\int_{\bar{S}_2} d^2\mathbf{a}\cdot\mathbf{F}_\pm\neq\int_{S_2} d^2\mathbf{a}\cdot\mathbf{F}_\pm. \tag{1.52}$$

The LHS approaches 2π as C_2 shrinks to zero; while the last integral approaches 0. The inequalities arise because the Stokes theorem fails if $\mathbf{A}$ is singular in the domain of surface integration. That is, to ensure the validity of the Stokes theorem, the area of integration cannot contain singular points. That is why we need to choose $\bar{S}_2$ for the loop C_2.

It is possible to remove the string of singularity if both types of gauges are used (Wu and Yang, 1975): people living on the northern hemisphere uses gauge-N, while people living on the southern hemisphere uses gauge-S (see Fig. 2(b)). So both tribes of people feel no singularity. However, they need to switch gauges near the equator with the gauge transformation,

$$\mathbf{A}^S_\pm(\mathbf{B})=\mathbf{A}^N_\pm(\mathbf{B})\pm\frac{\partial\phi}{\partial\mathbf{B}}. \tag{1.53}$$

In this case, the Stokes theorem can be applied for an integration over the whole sphere,

$$\begin{aligned}
&\int_{S^2} d^2\mathbf{a}\cdot\mathbf{F}_\pm\\
&=\int_{S_N} d^2\mathbf{a}\cdot\nabla\times\mathbf{A}^N_\pm+\int_{S_S} d^2\mathbf{a}\cdot\nabla\times\mathbf{A}^S_\pm && (1.54)\\
&=\oint_{C_\epsilon} d\boldsymbol{\ell}\cdot\mathbf{A}^N_\pm+\oint_{C_{-\epsilon}} d\mathbf{k}\cdot\mathbf{A}^S_\pm && (1.55)\\
&=\oint_{C_0} d\boldsymbol{\ell}\cdot\left(\mathbf{A}^N_\pm-\mathbf{A}^S_\pm\right) && (1.56)\\
&=\mp\oint_{C_0} d\boldsymbol{\ell}\cdot\frac{\partial\phi}{\partial\mathbf{B}}=\mp 2\pi. && (1.57)
\end{aligned}$$

In the line integrals, $C_{\pm\epsilon}$ are loops near the equator at angles $\theta=\pi/2\pm\epsilon$, and C_0 is the equator with the same orientation as C_ϵ.

Like the spin-1/2 system, the quantum Hall system also has non-trivial topology, and their Bloch states have similar non-trivial gauge structure. What is special about the QH Bloch state is that there exist nodal points in the BZ, where $u_{n\mathbf{k}_i}=0$. Similar to the south pole in Fig. 2(a), the phase is ambiguous at $\mathbf{k}_i$, and the Berry connection $\mathbf{A}_n(\mathbf{k})$ is singular there (see Fig. 3(a)). Assume there is only one singular point, then the line integral of $\mathbf{A}_n(\mathbf{k})$ around a small loop C enclosing $\mathbf{k}_1$ (and divided by 2π) equals the first Chern number (similar to the loop C_2 in Fig. 2(a)). It is sometimes called the **vorticity** of the singular point.

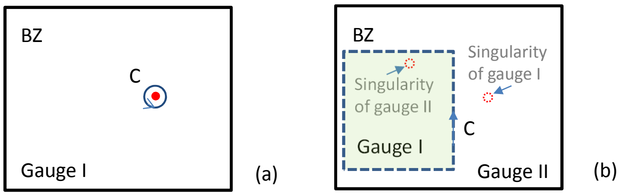

FIG. 3 (a) Gauge-I has a singularity at the red dot on the right side of the BZ. (b) An atlas with two patches of gauge is singularity-free. Gauge-I has a singularity on the right; gauge-II has one on the left.

Similarly, the singularity can be removed with multiple patches of gauge (Kohmoto, 1985): If $u^I_{n\mathbf{k}}$ are eigenstates of the Schrödinger equation, then

$$u^{II}_{n\mathbf{k}} = e^{i\chi_{n\mathbf{k}}} u^I_{n\mathbf{k}} \tag{1.58}$$

are also eigenstates. The phase factor $e^{i\chi_{n\mathbf{k}}}$ needs to be a single-valued function in $\mathbf{k}$, but is otherwise arbitrary. Their Berry connections are related by

$$\mathbf{A}^{II}_n(\mathbf{k}) = \mathbf{A}^I_n(\mathbf{k}) - \frac{\partial \chi_n(\mathbf{k})}{\partial \mathbf{k}}. \tag{1.59}$$

Assume gauge-I has a singularity on the right of the BZ; gauge-II has a singularity on the left of the BZ (see Fig. 3(b)). Then we can adopt gauge-I on the left side, and gauge-II on the right side, so that there is no singularity throughout the whole BZ. Again when crossing the boundary C between different patches, one needs to switch gauges using Eq. (1.59). The single-valuedness of $\chi_{\mathbf{k}}$ along the boundary would guarantee that the Berry curvature integrated over the whole BZ (and divided by 2π) is an integer value C_1 times 2π,

$$\begin{aligned}
&\int_{BZ} d^2\mathbf{k}\cdot \mathbf{F}_n \\
&= \int_{left} d^2\mathbf{k}\cdot \nabla\times \mathbf{A}^I_n + \int_{right} d^2\mathbf{k}\cdot\nabla\times\mathbf{A}^{II}_n \\
&= \oint_C d\mathbf{k}\cdot\left(\mathbf{A}^I_n - \mathbf{A}^{II}_n\right) \qquad (1.60)\\
&= \oint_C d\mathbf{k}\cdot \frac{\partial \chi_n}{\partial \mathbf{k}} = 2\pi\times\text{integer}. \qquad (1.61)
\end{aligned}$$

If there are multiple singularities for a single gauge, than more patches need be used, but the procedure remains essentially the same.

In addition to the two gauge choices above, one can also fix the phase of the Bloch state using the **parallel transport gauge** (see Thouless, 1984):

$$\left\langle u_{k_x0}\left|\frac{\partial}{\partial k_x}\right|u_{k_x0}\right\rangle = 0, \tag{1.62}$$
$$\left\langle u_{k_xk_y}\left|\frac{\partial}{\partial k_y}\right|u_{k_xk_y}\right\rangle = 0. \tag{1.63}$$

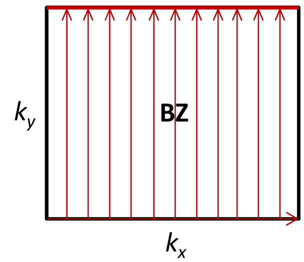

FIG. 4 Paths of parallel transport are indicated by lines with arrows.

The first equation defines the phase of the states (of a band n) on the k_x-axis; the second equation defines the phase along a line with fixed k_x (see Fig. 4). As a result, the phases of any two states in the BZ have a definite relation. Be aware that the phases defined by the parallel transport gauge are not necessarily single-valued.

The states on opposite sides of the BZ boundaries represent the same physical state. Therefore, they can only differ by a $\mathbf{k}$-dependent phase factor. Following Eqs. (1.62) and (1.63), we can choose

$$u_{k_x+g_x,k_y} = u_{k_xk_y}, \tag{1.64}$$
$$u_{k_x,k_y+g_y} = e^{i\delta(k_x)}u_{k_xk_y}, \tag{1.65}$$

where g_x and g_y are the basis of reciprocal lattice vectors. That is, the states on the opposite sides of the *vertical* boundaries have the same phase. The same cannot also be true for the *horizontal* boundaries, otherwise the topology will be too trivial to accommodate the quantum Hall conductivity.

Periodicity of the BZ requires that

$$\delta(k_x+g_x) = \delta(k_x) + 2\pi\times\text{integer}. \tag{1.66}$$

In order for the integral $(1/2\pi)\oint_{\partial BZ} d\mathbf{k}\cdot\mathbf{A}(\mathbf{k})$ (which is nonzero only along the *upper horizontal boundary*) to give the Hall conductivity C_1h/e^2, the integer in Eq. (1.66) obviously has to be equal to C_1.

Following the periodicity condition in Eq. (1.66), one can choose the phase to be,

$$\delta(k_x) = \tilde{\delta}(k_x) + C_1k_xa_1, \tag{1.67}$$

where $\tilde{\delta}(k_x+g_x) = \tilde{\delta}(k_x)$ is periodic in k_x, but otherwise remains arbitrary, a_1 is a lattice constant.

In summary, when the Bloch states have non-trivial topology, the phases of the Bloch states cannot be defined uniquely and smoothly over the whole BZ. There are either points of phase ambiguity, or lines where phases are not single-valued, so that the vorticity of the whole BZ can be non-zero (Soluyanov and Vanderbilt, 2012). This is the topological obstruction mentioned earlier.

Exercise

1. To derive Eq. (1.32), first write

$$|\Psi(t)\rangle = \sum_m e^{i\gamma_m(t)} e^{-\frac{i}{\hbar}\int_0^t dt' \varepsilon_{m\mathbf{k}(t')}} a_m(t)|u_{m\mathbf{k}}\rangle$$
$$= \sum_m e^{-\frac{i}{\hbar}\int_0^t dt' \varepsilon_{m\mathbf{k}(t')}} a_m(t)|\tilde{u}_{m\mathbf{k}}\rangle, \qquad (1.68)$$

in which $a_m(t)$ vary slowly with time. This is a multi-level generalization of Eq. (**??**) in Chap 2. Recall that $|\tilde{u}_{m\mathbf{k}}\rangle \equiv e^{i\gamma_m(t)}|u_{m\mathbf{k}}\rangle$ satisfies the parallel transport condition (see Prob. 2.1),

$$\langle \tilde{u}_{m\mathbf{k}}|\frac{\partial}{\partial t}|\tilde{u}_{m\mathbf{k}}\rangle = 0. \qquad (1.69)$$

(a) Use the Schrödinger equation $H|\Psi(t)\rangle = i\partial|\Psi(t)\rangle/\partial t$ and show that,

$$\frac{da_m(t)}{dt} = -e^{-\frac{i}{\hbar}\int_0^t dt'(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}})}\langle \tilde{u}_{m\mathbf{k}}|\frac{\partial}{\partial t}|\tilde{u}_{n\mathbf{k}}\rangle. \qquad (1.70)$$

(b) Assume the exponential factor oscillates much faster than the bracket, so that the latter can be treated as static. Integrate the equation above to get Eq. (1.32).
Note: If the non-integrable phases $\gamma_m(t)$ are *not* involved in a dynamical process, then they can be ignored and $|\tilde{u}_{m\mathbf{k}}\rangle$ are simplified as $|u_{m\mathbf{k}}\rangle$.
Ref: Appendix of Xiao *et al.*, 2010.

2. Under the one-band approximation, the effective Lagrangian of a Bloch wavepacket in an external electromagnetic field can be obtained by using the *time-dependent* variational principle. Here we merely take the effective Lagrangian as the starting point for subsequent derivations:

$$L(\mathbf{r},\mathbf{k};\dot{\mathbf{r}},\dot{\mathbf{k}}) \qquad (1.71)$$
$$= \hbar\mathbf{k}\cdot\dot{\mathbf{r}} + \hbar\dot{\mathbf{k}}\cdot\mathbf{A}(\mathbf{k}) - e\dot{\mathbf{r}}\cdot\mathbf{A}_e(\mathbf{r}) + e\phi_e - \varepsilon^m(\mathbf{r},\mathbf{k}),$$

where $\mathbf{A}(\mathbf{k})$ is the Berry connection, $\phi_e(\mathbf{r})$ and $\mathbf{A}_e(\mathbf{r})$ are the electromagnetic potentials, and $\varepsilon^m = \varepsilon(\mathbf{k}) - \mathbf{m}(\mathbf{k})\cdot\mathbf{B}$.

Treating *both* $\mathbf{r}$ and $\mathbf{k}$ as generalized *coordinates*, using the Euler-Lagrange equation to derive the equations of motion,

$$\hbar\dot{\mathbf{k}} = -e\mathbf{E} - e\dot{\mathbf{r}}\times\mathbf{B}, \qquad (1.72)$$
$$\hbar\dot{\mathbf{r}} = \frac{\partial\varepsilon^m}{\partial\mathbf{k}} - \hbar\dot{\mathbf{k}}\times\mathbf{F}, \qquad (1.73)$$

where $\mathbf{B} = \nabla_{\mathbf{r}}\times\mathbf{A}_e(\mathbf{r})$, and $\mathbf{F} = \nabla_{\mathbf{k}}\times\mathbf{A}(\mathbf{k})$.

For simplicity, assume that the electron is moving in the xy-plane and the magnetic field is along the z-direction. It would not be difficult to see that the equations of motion remain valid in more general situations.

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