

Berry curvature of Bloch state

- A. Basics of Bloch state
 - 1. Symmetries of Bloch state
- B. Electric response of Bloch state
- C. Quantized Hall conductivity
- D. Gauge choice of Bloch state

Basics

- (spinless) electron in a lattice

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



$$T_{\mathbf{R}}T_{\mathbf{R}'} = T_{\mathbf{R}'}T_{\mathbf{R}} = T_{\mathbf{R}+\mathbf{R}'}$$



$$c_{\mathbf{R}}c_{\mathbf{R}'} = c_{\mathbf{R}'}c_{\mathbf{R}} = c_{\mathbf{R}+\mathbf{R}'}$$

$$c_{\mathbf{R}} = e^{i\mathbf{k}\cdot\mathbf{R}}$$

- Lattice translation operator

$$T_{\mathbf{R}}\psi(\mathbf{r}) \equiv \psi(\mathbf{r} + \mathbf{R})$$

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

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

write

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



- Simultaneous eigenstates (Bloch states)

then

$$u_{\varepsilon\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{\varepsilon\mathbf{k}}(\mathbf{r}) \quad \text{Cell-periodic function}$$

$$\begin{cases} H\psi = \varepsilon\psi, \\ T_{\mathbf{R}}\psi = c_{\mathbf{R}}\psi, \quad |c_{\mathbf{R}}|=1 \end{cases}$$

- The Bloch wave differs from the plane wave of free electrons only by a periodic modulation.

- $u_{\varepsilon\mathbf{k}}(\mathbf{r})$ contains, in one unit cell, all info of $\psi_{\varepsilon\mathbf{k}}(\mathbf{r})$

Schroedinger eq. for $u_{\epsilon\mathbf{k}}(\mathbf{r})$

$$\tilde{H}_{\mathbf{k}}(\mathbf{r})u_{\epsilon\mathbf{k}} = \epsilon u_{\epsilon\mathbf{k}}$$

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

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

$$\therefore e^{i\mathbf{G}\cdot\mathbf{R}} = 1$$

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

Solve diff eq with with PBC

$$u_{\epsilon\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{\epsilon\mathbf{k}}(\mathbf{r})$$

➔ Discrete energy levels

$$\tilde{H}_{\mathbf{k}}(\mathbf{r})u_{n\mathbf{k}} = \epsilon_{n\mathbf{k}}u_{n\mathbf{k}}$$

Band index n ,
Bloch momentum \mathbf{k}

Since the two Bloch states $\psi_{n\mathbf{k}}$ and $\psi_{n\mathbf{k}+\mathbf{G}}$ satisfy the same Schrödinger equation (with $\epsilon_{n\mathbf{k}} = \epsilon_{n\mathbf{k}+\mathbf{G}}$) and the same boundary condition (Eqs. (1.16) and (1.17)), they can differ (for non-degenerate states) at most by a phase factor $\phi(\mathbf{k})$.

- Periodic gauge (choose $\phi(\mathbf{k})=0$)

$$\psi_{n\mathbf{k}+\mathbf{G}} = \psi_{n\mathbf{k}}$$

“Not applicable” to topological state (if no singularity is allowed), e.g., quantum Hall state (this is called **topological obstruction**)

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Berry curvature in Bloch state

- Cell-periodic Bloch state

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

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

- Berry connection

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

- Berry curvature

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

- Time reversal

$$u_{n\mathbf{k}}(\mathbf{r}) \rightarrow u_{n\mathbf{k}}^*(\mathbf{r}) = u_{n-\mathbf{k}}(\mathbf{r})$$

$$\begin{aligned}\therefore \mathbf{A}_n(\mathbf{k}) &\rightarrow i\langle u_{n-\mathbf{k}}^* | \frac{\partial}{\partial \mathbf{k}} | u_{n-\mathbf{k}}^* \rangle \\ &= -i\langle u_{n-\mathbf{k}} | \frac{\partial}{\partial \mathbf{k}} | u_{n-\mathbf{k}} \rangle = \mathbf{A}_n(-\mathbf{k})\end{aligned}$$

$$\mathbf{F}_n(\mathbf{k}) \rightarrow \nabla_{\mathbf{k}} \times \mathbf{A}_n(-\mathbf{k}) = -\mathbf{F}_n(-\mathbf{k})$$

- Space inversion

$$u_{n\mathbf{k}}(\mathbf{r}) \rightarrow u_{n\mathbf{k}}(-\mathbf{r}) = u_{n-\mathbf{k}}(-\mathbf{r})$$

$$\therefore \mathbf{A}_n(\mathbf{k}) \rightarrow i\langle u_{n-\mathbf{k}} | \frac{\partial}{\partial \mathbf{k}} | u_{n-\mathbf{k}} \rangle = -\mathbf{A}_n(-\mathbf{k})$$

$$\mathbf{F}_n(\mathbf{k}) \rightarrow \nabla_{\mathbf{k}} \times [-\mathbf{A}_n(-\mathbf{k})] = \mathbf{F}_n(-\mathbf{k})$$

- With both symmetries, (for non-degenerate state) the Berry curvature is zero.

Under **one-band approximation**
(same as the adiabatic approximation)

Velocity of electron in an electric field,

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

BC-induced velocity,
aka **anomalous velocity**

Pf. Choose **time-dependent gauge**

$$\mathbf{E} = -\partial \mathbf{A} / \partial t, \quad \mathbf{A} = -\mathbf{E}t$$

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

$$\mathbf{k}(t) = \mathbf{k}_0 - e \mathbf{E}t / \hbar.$$

To the 0-th order, just replace $|u_{n\mathbf{k}}\rangle$ with $|u_{n\mathbf{k}(t)}\rangle$

$$\text{and } \tilde{H}_{\mathbf{k}(t)} |u_{n\mathbf{k}(t)}\rangle = \varepsilon_{n\mathbf{k}(t)} |u_{n\mathbf{k}(t)}\rangle$$

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

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

Velocity of a
Bloch electron

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

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

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

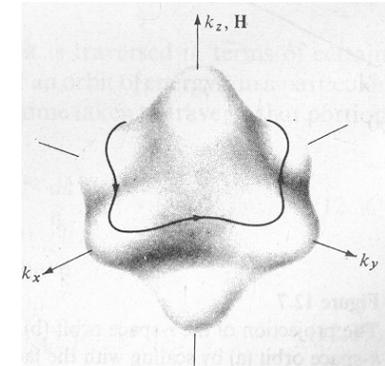
Recall **Semiclassical eq. of motion** (Ashcroft and Mermin, 1976)

Limits of validity: **one-band approximation** (Negligible inter-band transition)

$$\left\{ \begin{array}{l} \dot{\mathbf{r}} = \frac{\partial \varepsilon_{n\mathbf{k}}}{\hbar \partial \mathbf{k}} \\ \hbar \dot{\mathbf{k}} = -e\mathbf{E} - e\dot{\mathbf{r}} \times \mathbf{B} \end{array} \right. \quad \begin{array}{l} \bullet \text{ Lattice effect hidden in } E(k) \\ \bullet \text{ Derivation is non-trivial} \end{array}$$

Explains

- **Bloch oscillation** in a DC electric field
- **Cyclotron motion** in magnetic field
(after quantization, we have **de Haas-van Alphen effect**)



Update (see Xiao et al, 2010 RMP)

$$\left\{ \begin{array}{l} \dot{\mathbf{r}} = \frac{\partial \varepsilon_{n\mathbf{k}}^m}{\hbar \partial \mathbf{k}} - \dot{\mathbf{k}} \times \mathbf{F}_n \quad \text{Berry curvature} \\ \hbar \dot{\mathbf{k}} = -e\mathbf{E} - e\dot{\mathbf{r}} \times \mathbf{B}. \end{array} \right.$$

$$\varepsilon_{n\mathbf{k}}^m = \varepsilon_{n\mathbf{k}} - \mathbf{m}_n(\mathbf{k}) \cdot \mathbf{B}$$

Magnetic moment
of an electron (not
including spin)

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Mapping the Berry curvature from semiclassical dynamics in optical lattices

H. M. Price and N. R. Cooper

TCM Group, Cavendish Laboratory, J. J. Thomson Ave., Cambridge CB3 0HE, United Kingdom

An Aharonov-Bohm interferometer for determining Bloch band topology

L. Duca,^{1,2} T. Li,^{1,2} M. Reitter,^{1,2} I. Bloch,^{1,2} M. Schleier-Smith,³ U. Schneider^{1,2*}

Science 2015,
optical lattice

Experimental measurement of the Berry curvature from anomalous transport

Martin Wimmer^{1,2}, Hannah M. Price³, Iacopo Carusotto³ and Ulf Peschel^{2*}

Nat Phys 2017,
photonic system

Suppose we have a 2D electron system

- Current density

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



- Hall conductivity
($T=0$)

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

For a **filled band** n , the integral over F_n is an integer (proof later)

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

As a result, the Hall conductivity is quantized.

E.g., **Quantum Hall effect**, **Chern insulator** (anomalous Hall effect ch 5,

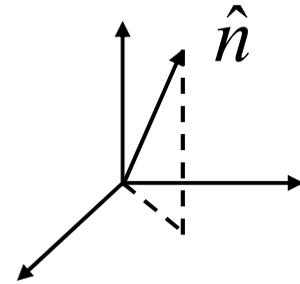
Haldance model ch 6)

~ lattice version of QHE

Before proving that C_1 is an integer, let's review the Berry curvature of a **spin-1/2 electron**:

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

(phase ϕ is ambiguous at $\theta=\pi$)

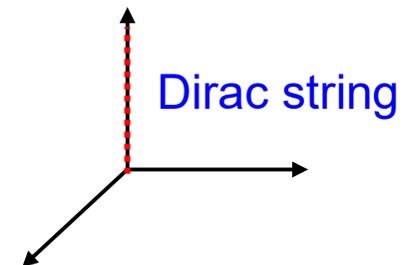
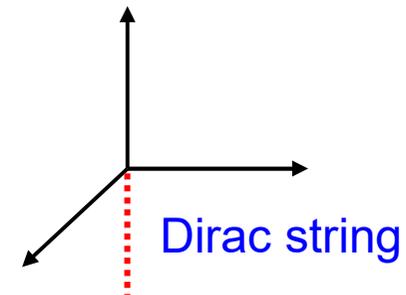


$$\rightarrow \mathbf{A}_{\pm}^N(\mathbf{B}) = \mp \frac{1}{2B} \frac{1 - \cos \theta}{\sin \theta} \hat{e}_{\phi} \quad \text{div at } \theta=\pi$$

$$|\hat{n}, \pm\rangle' = e^{\mp i\phi} |\hat{n}, \pm\rangle$$

$$\rightarrow \mathbf{A}_{\pm}^S(\mathbf{B}) = \pm \frac{1}{2B} \frac{1 + \cos \theta}{\sin \theta} \hat{e}_{\phi} \quad \text{div at } \theta=0$$

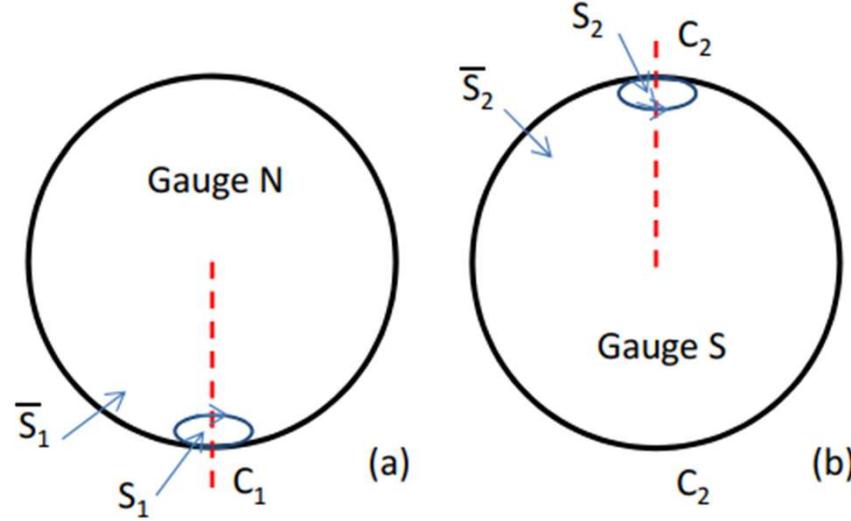
$$\mathbf{A}_{\pm}^S(\mathbf{B}) = \mathbf{A}_{\pm}^N(\mathbf{B}) \pm \frac{\partial \phi}{\partial \mathbf{B}}$$



The presence of the Dirac string is an example of the **topological obstruction**.

In Fig. 1 (a), (b), we see a loop C_1 near the south pole, and a loop C_2 near the north 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,

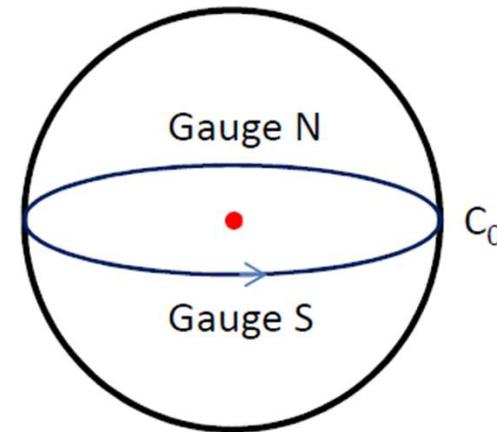
$$\oint_{C_1} d\ell \cdot \mathbf{A}_{\pm}^N = \int_{\bar{S}_1} d^2\mathbf{a} \cdot \mathbf{F}_{\pm} \simeq 2\pi \neq \int_{S_1} d^2\mathbf{a} \cdot \mathbf{F}_{\pm} \simeq 0$$



The LHS approaches 2π as C_1 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.

We can use two patches of gauge to avoid the singularity

$$\begin{aligned}
 &\rightarrow \int_{S^2} d^2 \mathbf{a} \cdot \mathbf{F}_{\pm} \\
 &= \int_{S_N} d^2 \mathbf{a} \cdot \nabla \times \mathbf{A}_{\pm}^N + \int_{S_S} d^2 \mathbf{a} \cdot \nabla \times \mathbf{A}_{\pm}^S \\
 &= \oint_{C_{\epsilon}} d\ell \cdot \mathbf{A}_{\pm}^N + \oint_{C_{-\epsilon}} d\mathbf{k} \cdot \mathbf{A}_{\pm}^S \\
 &= \oint_{C_0} d\ell \cdot (\mathbf{A}_{\pm}^N - \mathbf{A}_{\pm}^S) \\
 &= \mp \oint_{C_0} d\ell \cdot \frac{\partial \phi}{\partial \mathbf{B}} = \mp 2\pi.
 \end{aligned}$$

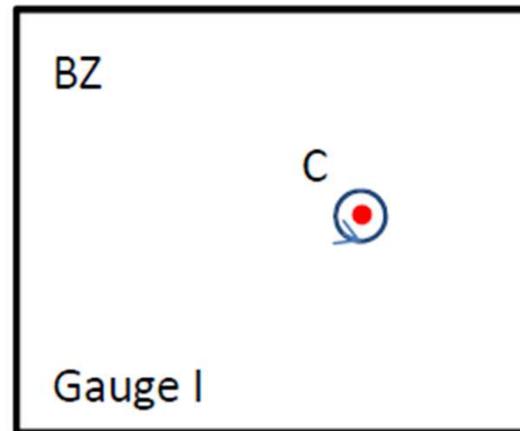


→ Total Berry flux is quantized.

The same analysis applies to the magnetic monopole in real space. So the flux, or **the magnetic charge of a magnetic monopole needs to be quantized** (Dirac 1931).

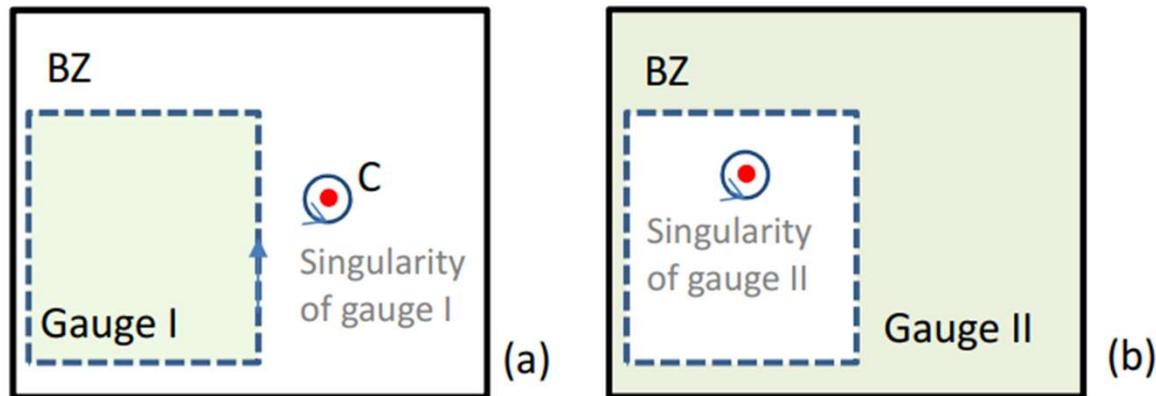
Now, back to the **quantum Hall system**

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.

- Gauge I: Demand $u_{n\vec{k}}(\vec{r}_1)$ to be real for some fixed \vec{r}_1 . This fixes the phase of $u_{n\vec{k}}(\vec{r}_1)$ for all \vec{k} , except at the point \vec{k}_1 when the cell-periodic function vanishes, and $\vec{A}_n(\vec{k}_1)$ is singular..
- Gauge II: Demand $u_{n\vec{k}}(\vec{r}_2)$ to be real for some fixed \vec{r}_2 . The cell-periodic function has a zero at some other point \vec{k}_2 .



- Around the boundary between two patches, we have

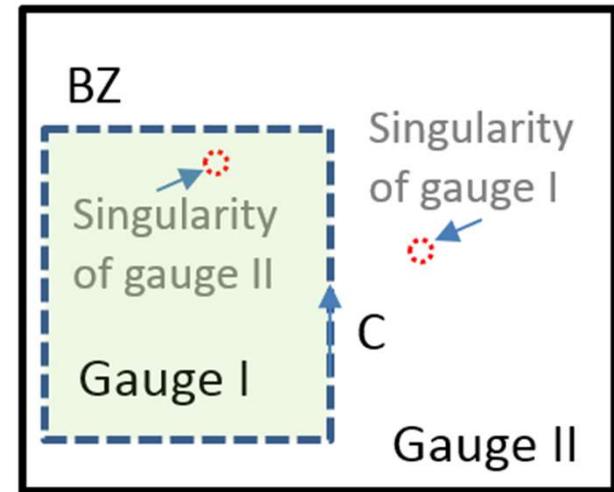
$$u_{n\mathbf{k}}^{II} = e^{i\chi_{n\mathbf{k}}} u_{n\mathbf{k}}^I \quad (\chi_{n\mathbf{k}} \text{ needs to be single-valued})$$

Kohmoto, Ann Phys 1985

$$C_1 = \frac{1}{2\pi} \int_{BZ} d^2k F_z(\vec{k}) \quad \text{is an integer}$$

Pf: $u_{n\mathbf{k}}^{II} = e^{i\chi_{n\mathbf{k}}} u_{n\mathbf{k}}^I$ Gauge transformation

$$\rightarrow \mathbf{A}_n^{II}(\mathbf{k}) = \mathbf{A}_n^I(\mathbf{k}) - \frac{\partial \chi_n(\mathbf{k})}{\partial \mathbf{k}}$$



Using two patches of gauge to avoid singularity

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

This conclusion remains valid for systems with disorder and electron interaction (Niu-Thouless-Wu PRB 1985).