I. Berry curvature of Bloch states
   A. Basics
   B. Quantum Hall effect
   C. Gauge choice of Bloch state

Review:

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

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

Symmetry:

Space inversion

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

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

Time reversal

$$u_{n\mathbf{k}}(\mathbf{r}) \;\rightarrow\; u^*_{n\mathbf{k}}(\mathbf{r})[= u_{n-\mathbf{k}}(\mathbf{r})] = u_{n\mathbf{k}}(\mathbf{r}),$$

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

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

Velocity of electron in an electric field,

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

Pf: Choose time-dependent gauge

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

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

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

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

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),

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

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

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

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

Current density

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

Hall conductivity
(T=0)

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

For a filled band n, the integral over F_n is an integer

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.

>> Quantum Hall effect

The topology in quantum Hall effect

Quantized Hall Conductance in a Two-Dimensional Periodic Potential

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Department of Physics, University of Washington, Seattle, Washington 98195
(Received 30 April 1982)

The Hall conductance of a two-dimensional electron gas has been studied in a uniform magnetic field and a periodic substrate potential U. The Kubo formula is written in a form that makes apparent the quantization when the Fermi energy lies in a gap. Explicit expressions have been obtained for the Hall conductance for both large and small $U/\hbar\omega_c$.

PACS numbers: 72.15.Gd, 72.20. Mg, 73.90.+b

Hall conductivity for the *n*-th band

$$(\sigma_H)_n = \frac{e^2}{h}\left[\frac{1}{2\pi}\int_{BZ} d^2k\, F_{nz}(\vec{k})\right]$$

$$= \frac{e^2}{h} C_1$$

1st Chern number (an integer for a filled band, proved later)

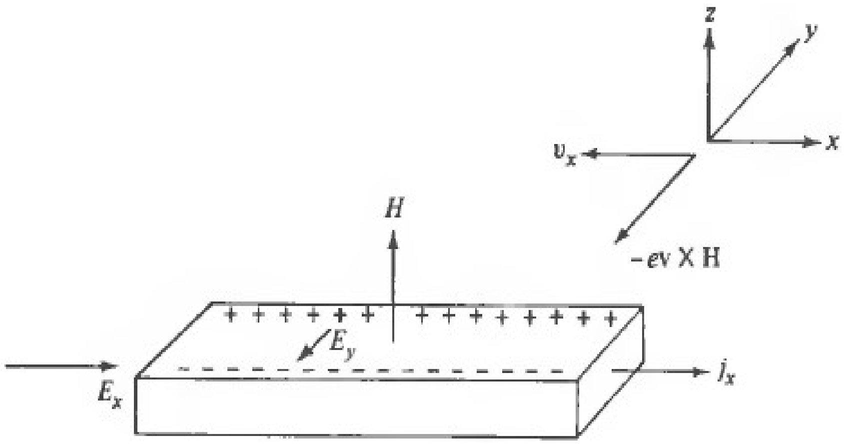
$$C_1 \equiv \frac{1}{2\pi}\int_{BZ} d^2k\, F_{nz}(\vec{k})$$

2016

First, classical Hall effect (1879)

$$m^* \frac{d\vec{v}}{dt} = -e\vec{E} - e\vec{v}\times\vec{B} - m^*\frac{\vec{v}}{\tau}$$

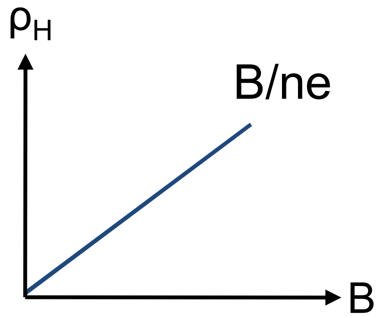
$$\vec{B} = B\hat{z};\ d\vec{v}/dt = \vec{0} \text{ at steady state}$$



$$\Rightarrow \begin{pmatrix} m^*/\tau & eB \\ -eB & m^*/\tau \end{pmatrix}\begin{pmatrix} v_x \\ v_y \end{pmatrix} = -e\begin{pmatrix} E_x \\ E_y \end{pmatrix}$$

$$\vec{j} = -en\vec{v}$$

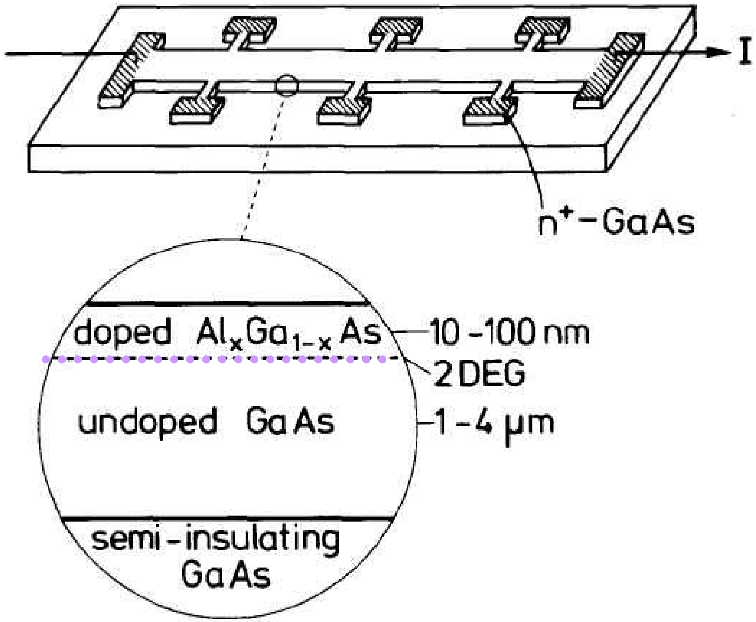
$$\Rightarrow \begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} \frac{m^*}{ne^2\tau} & \frac{B}{ne} \\ -\frac{B}{ne} & \frac{m^*}{ne^2\tau} \end{pmatrix}\begin{pmatrix} j_x \\ j_y \end{pmatrix} = \rho_0\begin{pmatrix} 1 & \omega_c\tau \\ -\omega_c\tau & 1 \end{pmatrix}\begin{pmatrix} j_x \\ j_y \end{pmatrix}$$



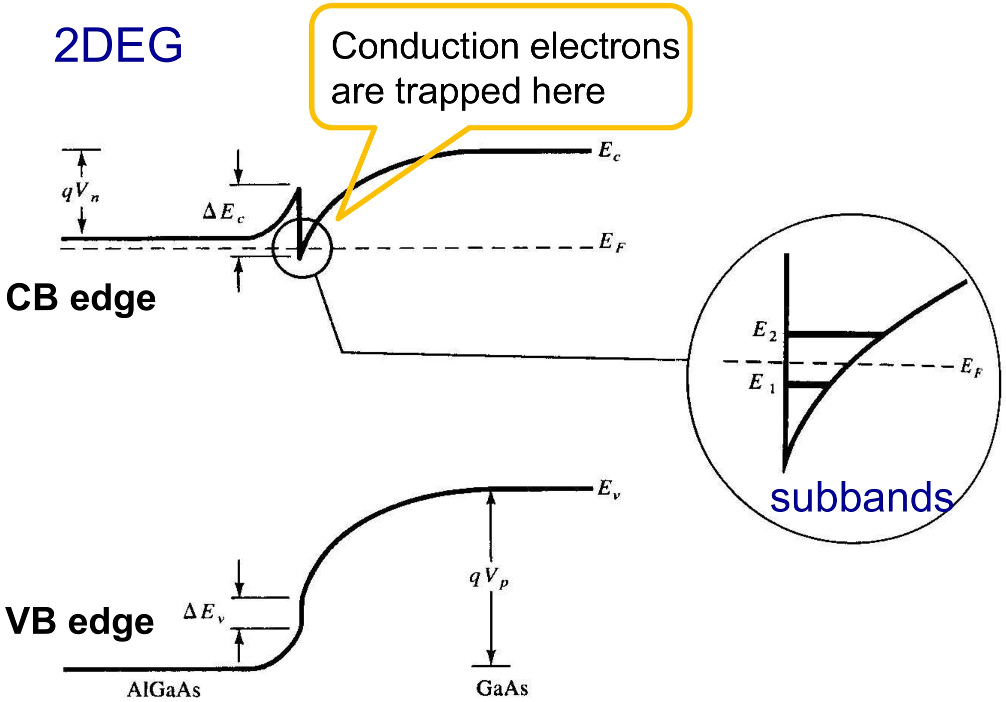
$$\rho_0 = \frac{m^*}{ne^2\tau},\ \omega_c = \frac{eB}{m^*}$$

Hall effect in 2-dimensional electron gas (2DEG)

GaAs/AlGaAs heterojunction

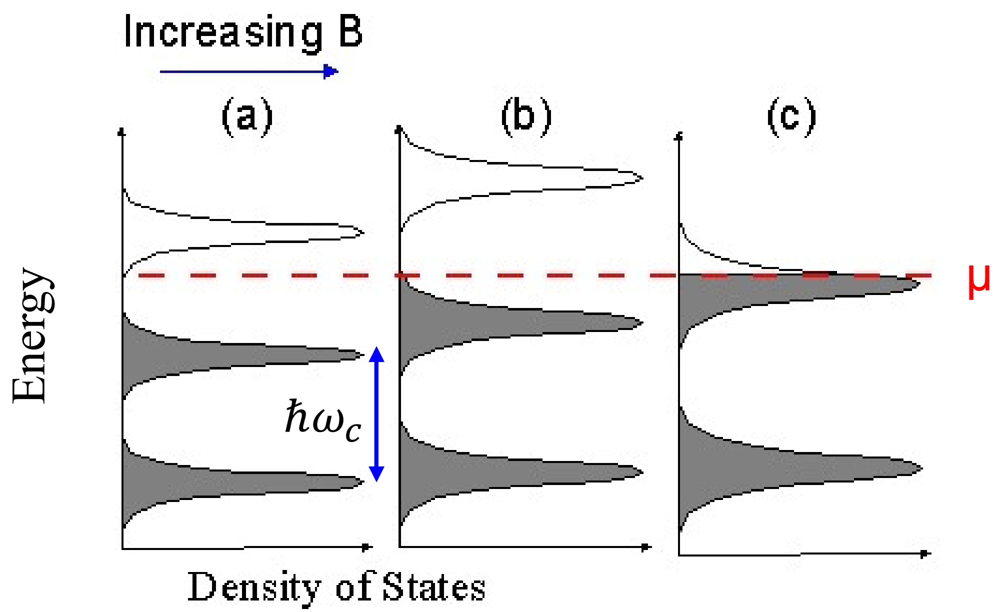


2DEG



- At low T, the dynamics along z-direction is frozen in the ground state → 2DEG
- Apply a strong B field, then there are Landau levels (LLs)

Landau levels
(LLs)



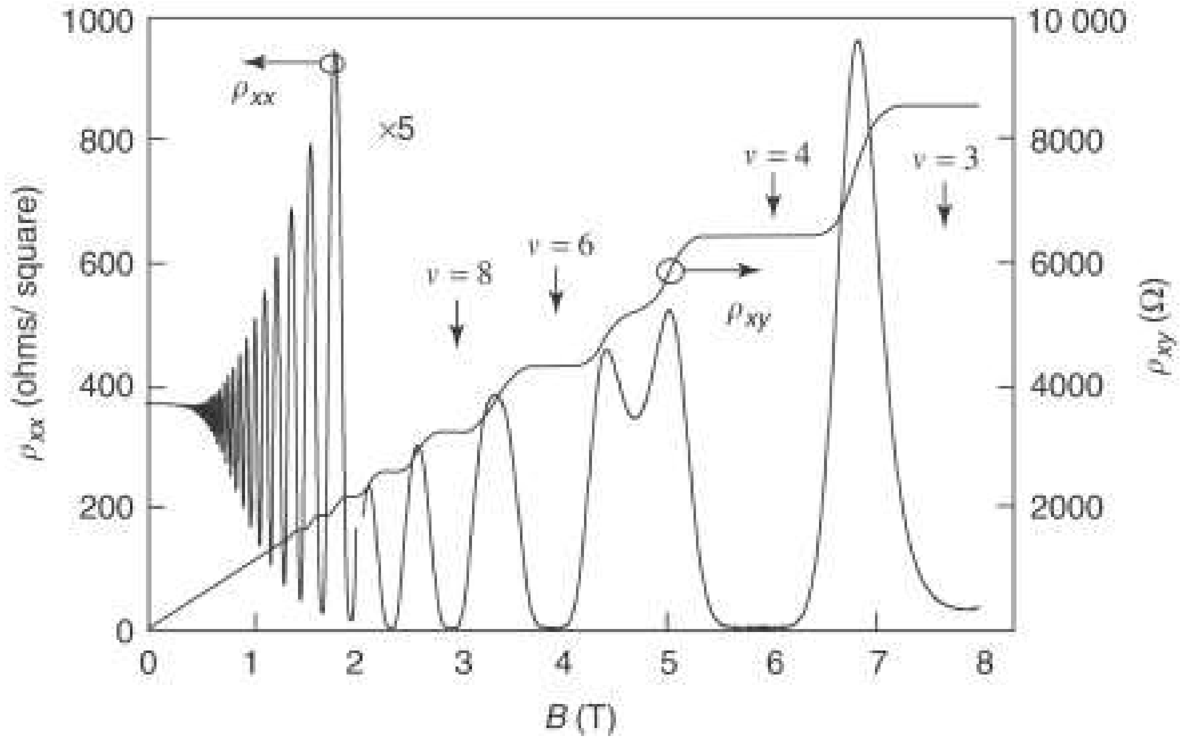
Cyclotron energy

$$\hbar\omega_c = 1.16H \times 10^{-8}\,\mathrm{eV} \times \frac{m}{m^*}$$
$$= 1.34H \times 10^{-4}\,\mathrm{K}$$

(*H* in Gauss) (for GaAs, m*=0.067m)

- Landau levels have non-zero Chern numbers
- Hall conductance is quantized whenever the Fermi energy lies inside an energy gap

[Integer] Quantum Hall effect (von Klitzing, 1980)



1985

Hall resistivity and conductivity at plateaus

$$\rho_H = \frac{1}{n}\frac{h}{e^2}$$

$$\sigma_H = n\frac{e^2}{h}$$

h/e^2 = 25.81280745 k-ohm

accurate to 10^{-9}, a defined value after 1990

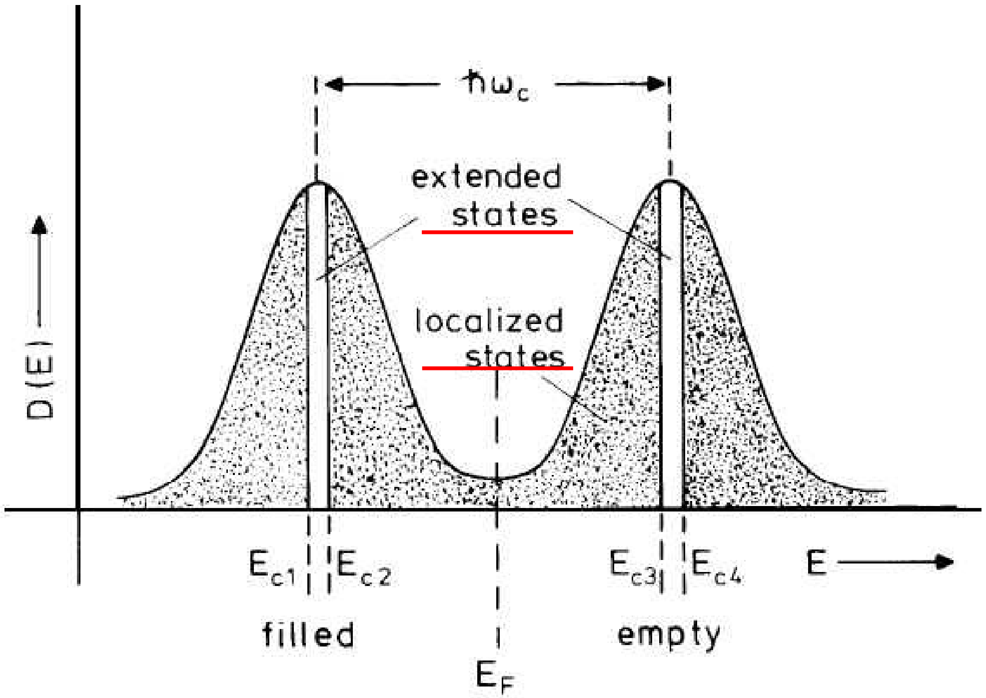
fine structure constant, $\alpha \equiv e^2/4\pi\varepsilon_0\hbar c$.

[Note: After 2019, the values of e, h, and c are defined, and only ε_0 is uncertain.]

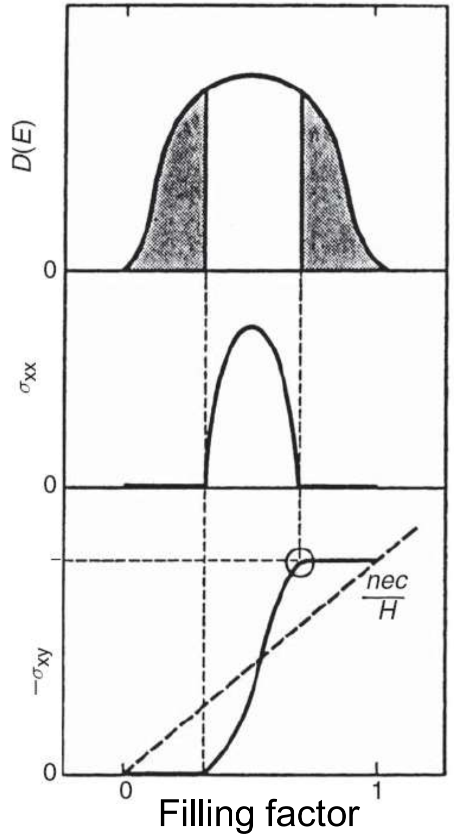
Disorders and Hall plateaus

(there is no plateaus in a clean 2DEG)

Broadened LLs



Aoki, CMST 2011



To observe IQHE, we need

- Two-dimensional electron system
- The breaking of time-reversal symmetry
- Filled energy bands (insulator) with non-zero Chern numbers
  - Landau levels (IQHE)
  - Bands with magnetization (QAHE) ← next chap

(Low temp, high B field are usually required)

Examples of Macroscopic Quantum Phenomena

- Superconductivity (Onnes, 1911)
- Superfluidity (Kapitsa, 1937)
- Quantum Hall effect (von Klitzing, 1980)
- Bose-Einstein condensation (Cornell and Wieman, 1995)
- …

Quantum Hall Effect in 2D systems

Need to break time-reversal symmetry

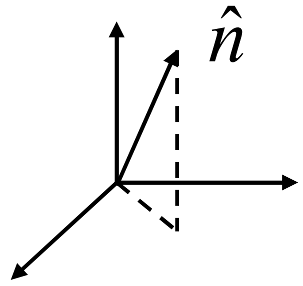
- Si MOSFET (von Klitzing et al, 1980)
- GaAs heterojunction (Stormer, 1982)
- Graphene (Novoselov, Science 2007)
- Polar oxide heterostructures (Tsukazaki et al, Science 2007)
- Twisted bilayer graphene (Lee et al, PRL 2011)
- TMD: WSe_2 (Movva et al, PRL 2017)
- InSe (Bandurin et al, Nat Nanotech 2017)
- Tellurene (Qiu et al, Nat Nanotech 2020)
- Twisted Bilayer $MoTe_2$ (Cai et al, Nature 2023)

…

Transition Metal Dichalcogenide
過渡金屬硫化物

Before introducing the proof that C_1 is an integer,

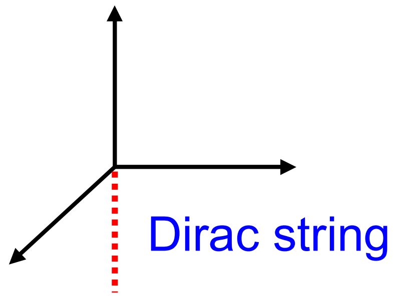
let's review the Berry curvature of a spin-1/2 electron:



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

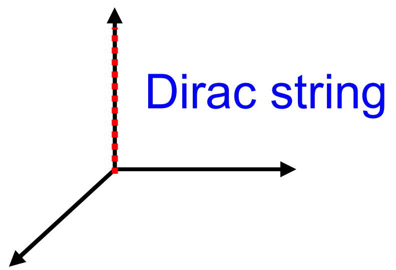
(phase ϕ is ambiguous at $\theta=\pi$)

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



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

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



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

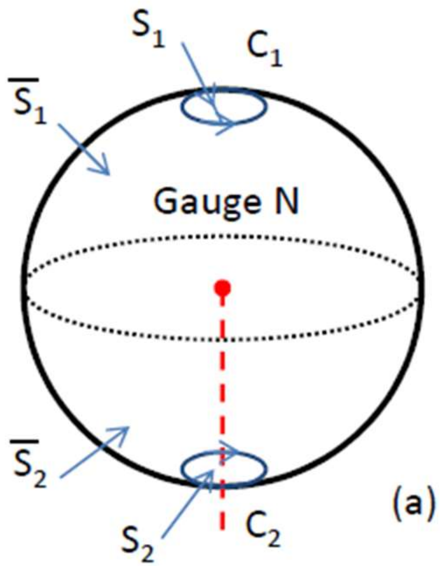
The presence of the Dirac string is an example

of the topological obstruction.

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,

$$\oint_{C_2} d\boldsymbol{\ell} \cdot \mathbf{A}^N_{\pm} = \int_{\bar{S}_2} d^2\mathbf{a} \cdot \mathbf{F}_{\pm} \neq \int_{S_2} d^2\mathbf{a} \cdot \mathbf{F}_{\pm}. \qquad (1.36)$$

Vorticity of the singularity



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.

We can use two patches of gauge to avoid the singularity

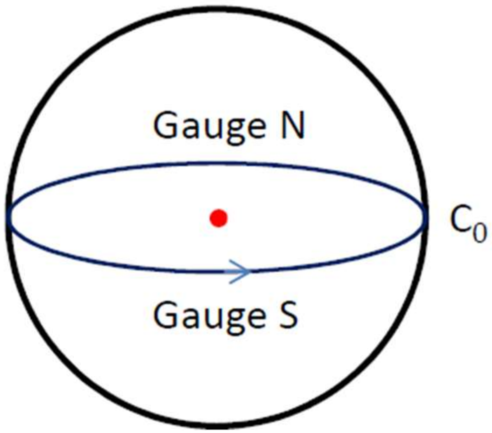
$$\int_{S^2} d^2\mathbf{a} \cdot \mathbf{F}_\pm$$

$$= \int_{S_N} d^2\mathbf{a} \cdot \nabla \times \mathbf{A}_\pm^N + \int_{S_S} d^2\mathbf{a} \cdot \nabla \times \mathbf{A}_\pm^S$$

$$= \oint_{C_\epsilon} d\boldsymbol{\ell} \cdot \mathbf{A}_\pm^N + \oint_{C_{-\epsilon}} d\mathbf{k} \cdot \mathbf{A}_\pm^S$$

$$= \oint_{C_0} d\boldsymbol{\ell} \cdot (\mathbf{A}_\pm^N - \mathbf{A}_\pm^S)$$

$$= \mp \oint_{C_0} d\boldsymbol{\ell} \cdot \frac{\partial \phi}{\partial \mathbf{B}} = \mp 2\pi.$$



Total Berry flux is quantized.

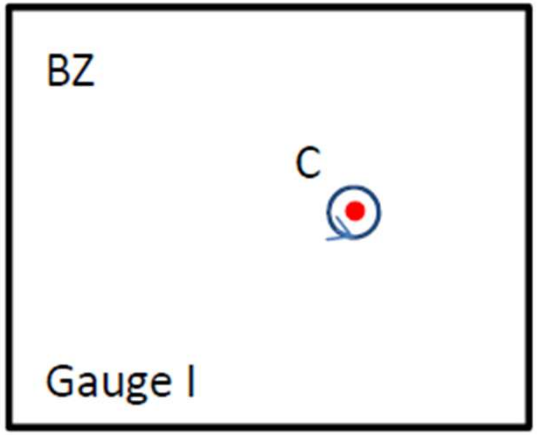
The same analysis applies to the magnetic monopole in real space.

So the flux of a magnetic monopole (or the monopole charge)

needs be quantized.

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)).

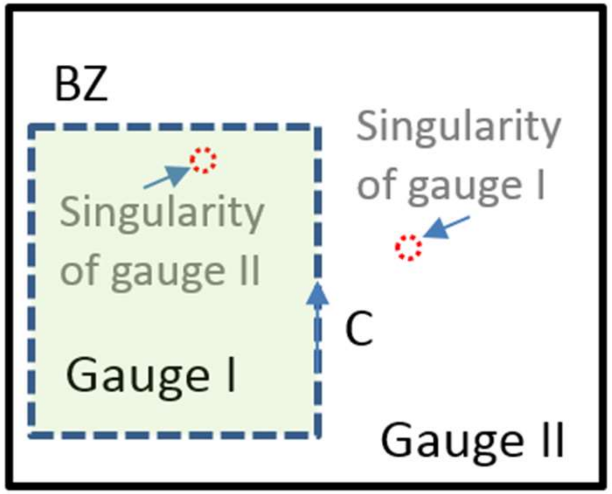


Assume there is only one singular point, then the line integral of $\mathbf{A}_n(\mathbf{k})$ around a small loop C enclosing $\mathbf{k}_1$ (and divided by 2π) equals the first Chern number (similar to the loop C_2 in Fig. 2(a)). It is sometimes called the **vorticity** of the singular point.

$$C_1 = \frac{1}{2\pi} \int_{BZ} d^2k \, F_z(\vec{k})$$ 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

$$\Rightarrow \int_{BZ} d^2\mathbf{k} \cdot \mathbf{F}_n$$

$$= \int_{left} d^2\mathbf{k} \cdot \nabla \times \mathbf{A}_n^{I} + \int_{right} d^2\mathbf{k} \cdot \nabla \times \mathbf{A}_n^{II}$$

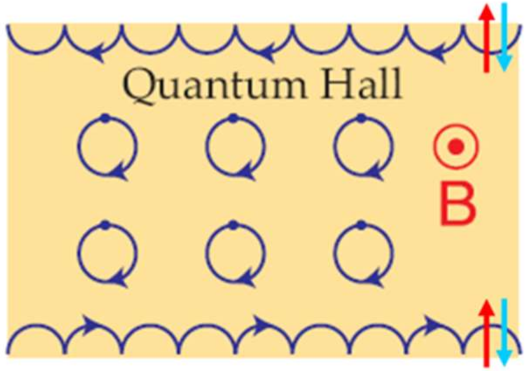
$$= \oint_C d\mathbf{k} \cdot (\mathbf{A}_n^{I} - \mathbf{A}_n^{II})$$

$$= \oint_C d\mathbf{k} \cdot \frac{\partial \chi_n}{\partial \mathbf{k}} = 2\pi \times \text{integer}.$$

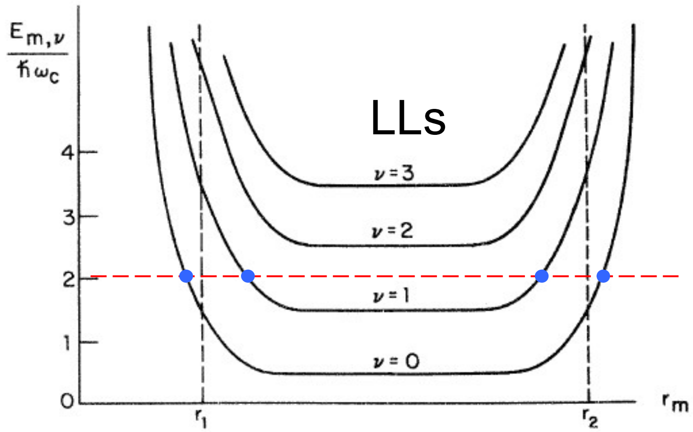
Robust Edge state in quantum Hall insulator

3 levels of understanding

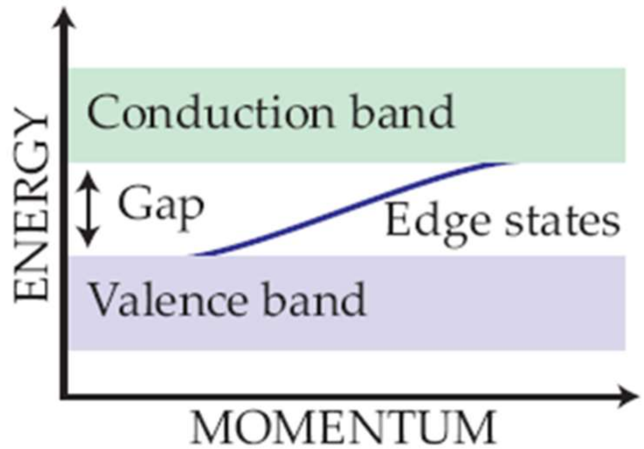
1. Classical — Skipping orbit (chiral)



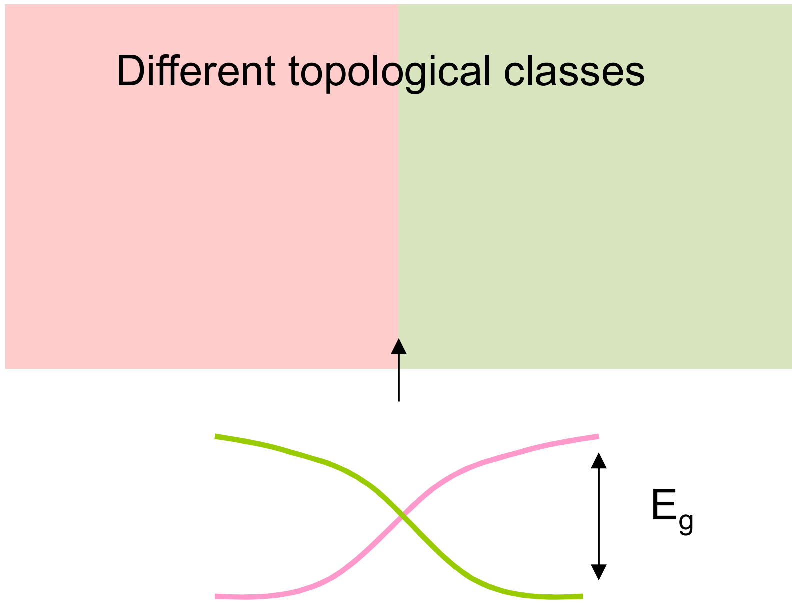
2. Semiclassical — Bending of LLs near boundary



3. Quantum — Energy levels of edge state appear within an energy gap



Bulk-edge correspondence in topological materials



Semiclassical picture:
energy levels must cross each other near the interface (otherwise the topology won't change).

→ gapless states bound to the interface, which are protected by topology.

- No general proof, but (for non-interacting electrons).no counter example either.