Berry curvature of Bloch states

A. Basics of Bloch state

B. Electric response of Bloch state

C. Quantum Hall effect

D. Gauge choice of Bloch state

Basics

- Lattice Hamiltonian

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

- Lattice translation operator

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

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

- Simultaneous eigenstates (Bloch states)

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

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

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

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

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

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

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

- The Bloch wave differs from the plane wave of free electrons only by a periodic modulation.
- $u_{\varepsilon\mathbf{k}}(\boldsymbol{r})$ contains, in one unit cell, all info of $\psi_{\varepsilon\mathbf{k}}(\mathbf{r})$

Schroedinger eq. for $u_{\varepsilon \boldsymbol{k}}(\boldsymbol{r})$

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

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

Solve diff eq with with PBC

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

➡ Discrete energy levels

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

Band index n,
Bloch momentum $\boldsymbol{k}$

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

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

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

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 $\phi(\mathbf{k})$.

- Periodic gauge (choose $f(k)$=0)

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

Not applicable to topological state, e.g., quantum Hall state (this is called topological obstruction)

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

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

- 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

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

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

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

Velocity of electron in an electric field,

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

BC-induced velocity,

aka anomalous velocity

Pf: Choose time-dependent gauge

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

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

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

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),

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

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

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

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

- Current density

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

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

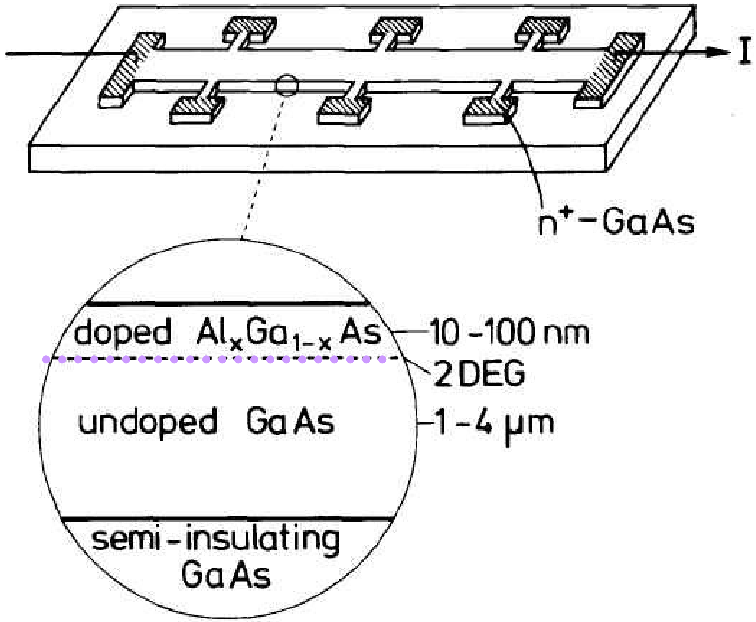
As a result, the Hall conductivity is quantized.

E.g., Quantum Hall effect, Chern insulator (anomalous Hall effect ch 5, Haldance model ch 6)

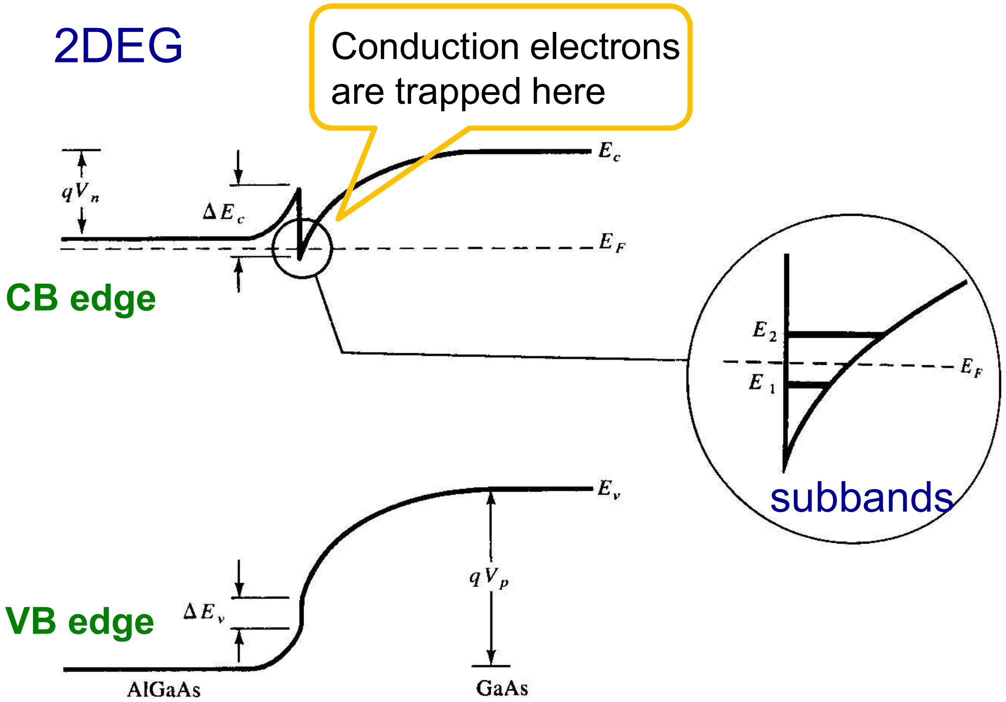
~ lattice version of QHE

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

GaAs/AlGaAs heterojunction

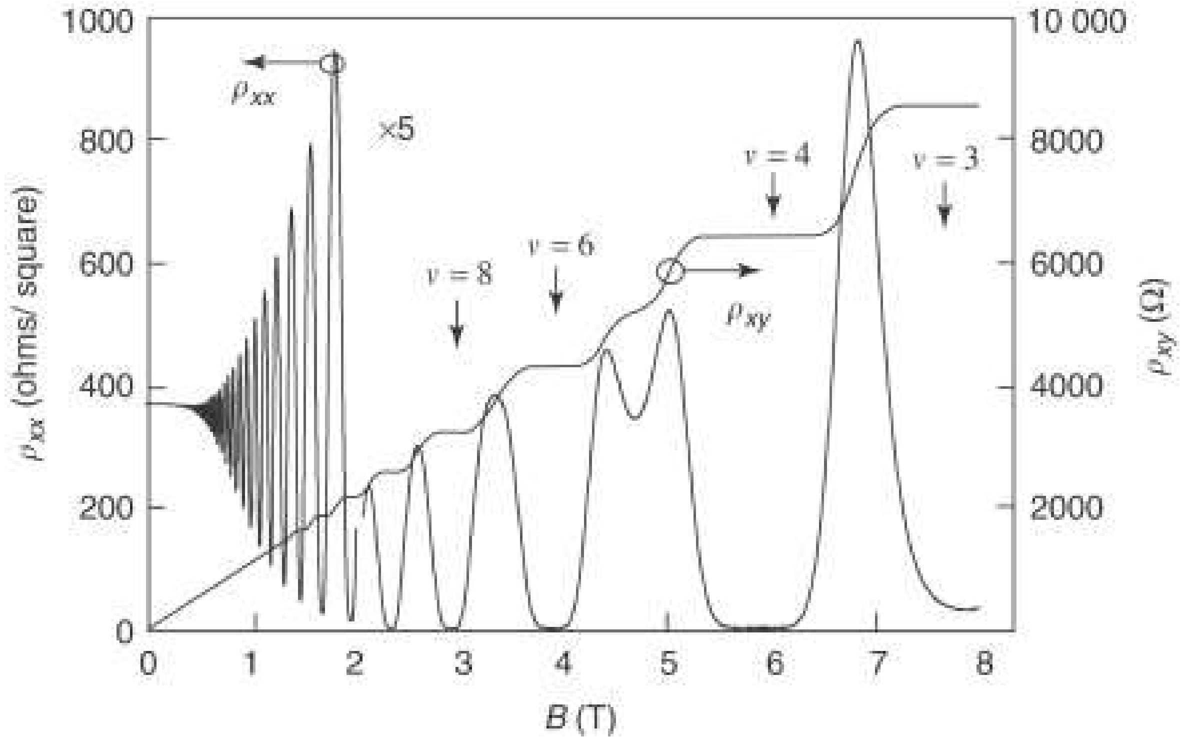


2DEG



- 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)

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



1985

Hall resistivity and Hall 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

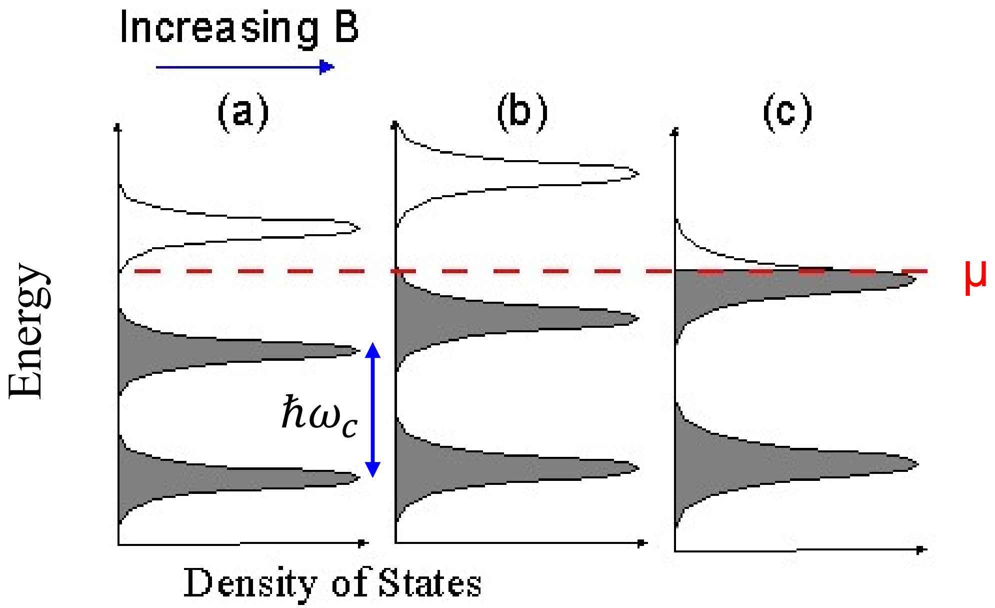
accurate to 10^{-9}, a defined value after 1990

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.]

Brief explanation of the QHE:

Landau levels
(LLs)



Cyclotron energy

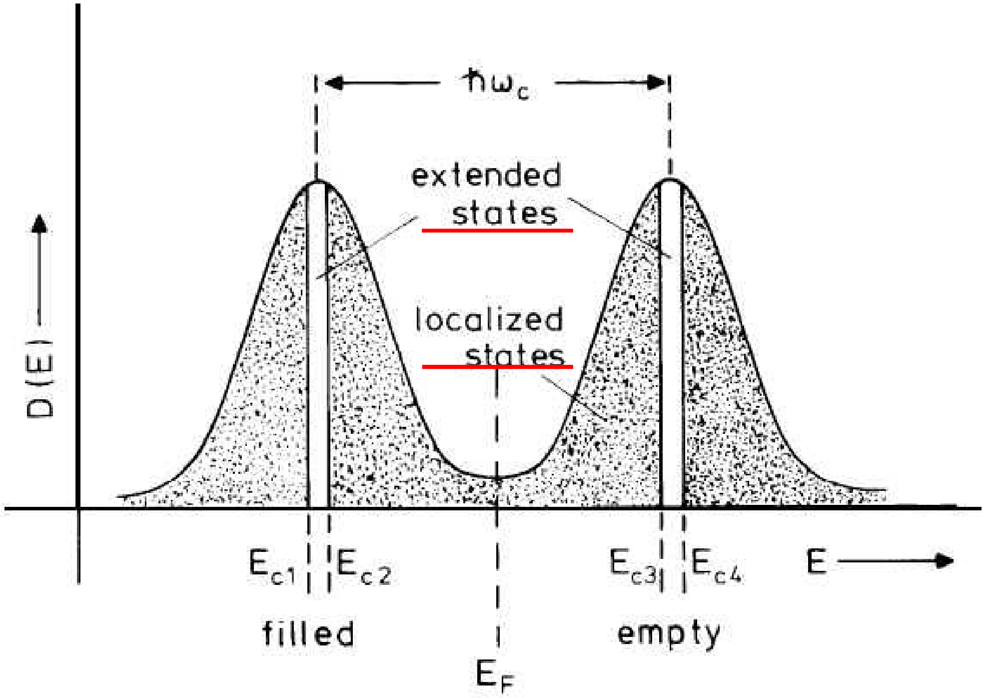
$$\hbar\omega_c = 1.16H \times 10^{-8}\,\text{eV} \times \frac{m}{m^*}$$
$$= 1.34H \times 10^{-4}\,\text{K}$$

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

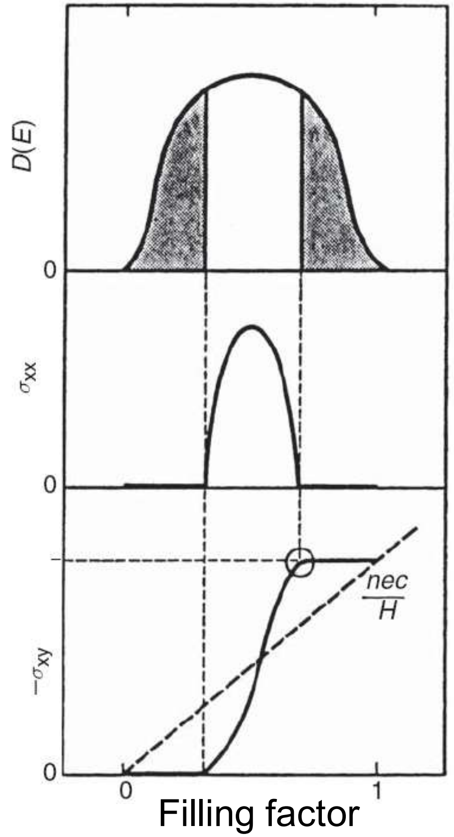
- Landau levels have non-zero Chern numbers
- Hall conductance is quantized whenever the Fermi energy lies inside an energy gap

Disorders and Hall plateaus

LLs are broadened due to disorders



Aoki, CMST 2011



(there is no plateaus in a clean 2DEG)

To observe IQHE, we need

- Two-dimensional electron system
- Breaking 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, but not necessarily, required)

Examples of Macroscopic Quantum Phenomena

- Superconductivity (Onnes, 1911)
- Superfluidity (Kapitsa, 1937)
- Quantum Hall effect (von Klitzing, 1980) < room temperature possible
- 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)
- …

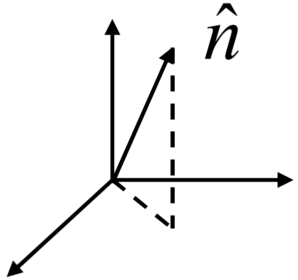
Transition Metal Dichalcogenide

過渡金屬硫化物

Before proving that C_1 is an integer, let's review

the Berry curvature of a spin-1/2 electron:

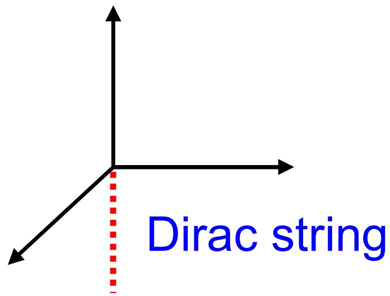
$$|\hat{n},+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}, \; |\hat{n},-\rangle = \begin{pmatrix} -e^{-i\phi}\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix}.$$



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

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

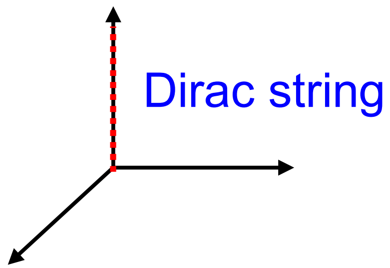
div at $\theta=\pi$



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

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

div at $\theta=0$



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

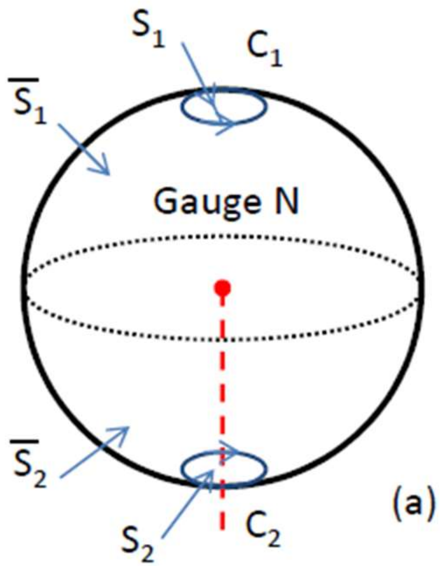
The presence of the Dirac string is an example

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,

$$\oint_{C_2} d\boldsymbol{\ell} \cdot \mathbf{A}_{\pm}^{N} = \overbrace{\int_{\bar{S}_2} d^2\mathbf{a} \cdot \mathbf{F}_{\pm}}^{\simeq 2\pi} \neq \overbrace{\int_{S_2} d^2\mathbf{a} \cdot \mathbf{F}_{\pm}}^{\simeq 0}. \qquad (1.36)$$

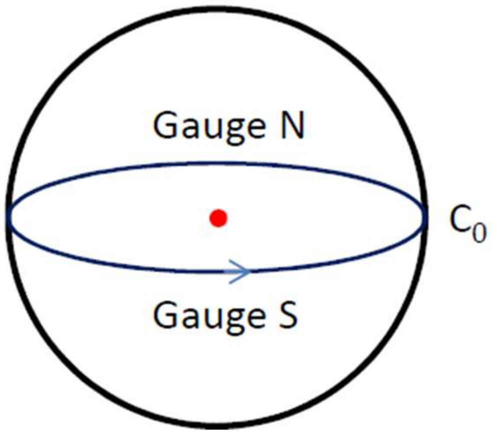
Vorticity of the singularity



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

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



Total Berry flux is quantized.

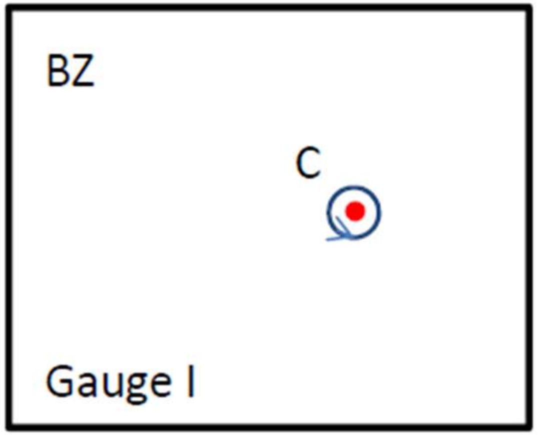
The same analysis applies to the magnetic monopole in real space.

So the flux 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.

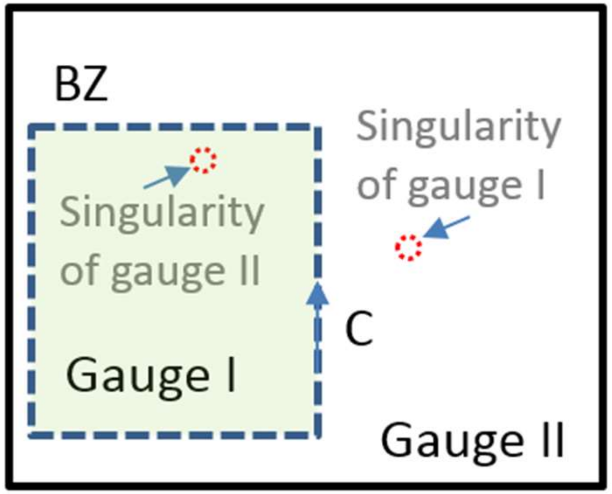
$$C_1 = \frac{1}{2\pi}\int_{BZ} d^2k\, F_z(\vec{k})$$ is an integer

Single-valued

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

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

Using two patches of gauge to avoid singularity



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