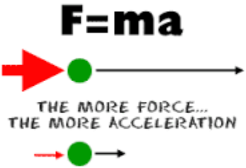
Quantum many-body systems (8.513 fa19) Lecture note 1

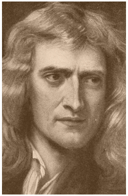
Xiao-Gang Wen

https://stellar.mit.edu/S/course/8/fa19/8.513/index.html

Classical motion of a particle and Newton's Law

The motion of electrons or holes in a semiconductor does not follow Newton's law. They follow a generalized Newton law.





First-order equation of motion and phase-space Lagrangian

- If (x, p) fully characterize the state of a particle, then their equation of motion is first-order:

$$\dot{x} = \partial_p H(x, p), \quad \dot{p} = -\partial_x H(x, p)$$ Why this form?

which can be obtained via phase-space Lagrangian

$$\mathcal{L}(x, \dot{x}, p, \dot{p}) = p\dot{x} - H(x, p), \quad S = \int \mathrm{d}t \; \mathcal{L}(x, \dot{x}, p, \dot{p}).$$

- A classical system is fully characterized by 1) **EOM + Hamiltonian**, or by 2) **phase-space Lagrangian**.
- A phase-space point fully characterises a classical state.
- Phase-space Lagrangian contains only first order time derivative.
- From S to first-order equation of motion

$$\delta S = \int \mathrm{d}t \; \delta p \underbrace{[\dot{x} - \partial_p H(x, p)]}_{=0} + \delta x \underbrace{[-\dot{p} - \partial_x H(x, p)]}_{=0},$$

we got that above equation of motion.

Phase-space Lagrangian description of Shrödinger equation

For a quantum system, its state is fully characterized by a vector $\phi\rangle$ in a Hilbert space $\mathcal{V}$:

$$|\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \end{pmatrix}, \to \quad \text{first-order E.O.M} \quad \mathrm{i}\hbar\dot{\phi}_m = H_{mn}\phi_n$$

(Why ϕ_m is complex? Why $|\phi_m|^2$ related to probability?)

- Phase-space Lagrangian

$$L = \mathrm{i}\hbar\phi_m^*\dot{\phi}_m - \phi_m^* H_{mn}\phi_n = \langle\phi|\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t} - H|\phi\rangle, \qquad S = \int \mathrm{d}t\ L.$$

- From (*Can we have non-linear Shrödinger equation?*)

$$\delta S = \int \mathrm{d}t\ \delta\phi_m^*[\mathrm{i}\hbar\dot{\phi}_m - H_{mn}\phi_n] + \delta\phi_n[-\mathrm{i}\hbar\dot{\phi}_m^* - \phi_m^* H_{mn}]$$

we get the equation of motion

$$\mathrm{i}\hbar\dot{\phi}_m = H_{mn}\phi_n, \qquad -\mathrm{i}\hbar\dot{\phi}_n^* = \phi_m^* H_{mn}.$$

Dynamical variational approach

- Given a Hamiltonian H, we can use variational approach to get an approximate ground state, by minimizing $\langle\phi_{\xi^I}|H|\phi_{\xi^I}\rangle$, where ξ^I are the variational parameters → approximate ground state $|\phi_{\xi^I_0}\rangle$.
  But how to get the low energy excited states?
- **Dynamical variational approach** (semi-classical approach):

- we assume the variational parameters has a time-dependence $\xi^I(t)$.
- The variational parameters ξ^I fully characterize the state, *ie* ξ^I parametrize a phase-space.
- The dynamics of $\xi^I(t)$ is given by the phase-space Lagrangian

$$\mathcal{L}(\xi^I, \dot{\xi}^I) = \langle\phi_{\xi^I(t)}|\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t} - H|\phi_{\xi^I(t)}\rangle = \hbar a_I(\xi^I)\dot{\xi}^I - \bar{H}(\xi^I)$$

where

$$a_I(\xi^I) \equiv \mathrm{i}\langle\phi_{\xi^I}|\partial_{\xi^I}|\phi_{\xi^I}\rangle,$$

which is the **vector potential** in the phase-space.

Most general phase-space description of classical system

From $S = \int \mathrm{d}t\ L(\dot{\xi}^I, \xi^I) = \int \mathrm{d}t\ [\hbar a_I \dot{\xi}^I - \bar{H}]$, we get

$$\delta S = \int \mathrm{d}t\ [\hbar(\partial_J a_I)\delta\xi^J \dot{\xi}^I - \hbar \dot{a}_I \delta\xi^I - \delta\xi^I \partial_I \bar{H}(\xi^I)]$$

$$= \int \mathrm{d}t\ \delta\xi^I [\hbar(\partial_I a_J)\dot{\xi}^J - \hbar(\partial_J a_I)\dot{\xi}^J - \partial_I \bar{H}] = \int \mathrm{d}t\ \delta\xi^I [\hbar b_{IJ} \dot{\xi}^J - \partial_I \bar{H}]$$

and the equation of motion

$$\hbar b_{IJ} \dot{\xi}^J = \frac{\partial \bar{H}}{\partial \xi^I}, \qquad b_{IJ} = \partial_I a_J - \partial_J a_I = \text{“magnetic field” in phase-space}$$

- The above EOM conserve energy $\partial_t \bar{H}(\xi^I(t)) = 0$.

- **Gauge redundancy**: we may choose an equivalent (redundant) trial wave function $\mathrm{e}^{\mathrm{i}\theta(\xi^I)}|\psi_{\xi^I}\rangle$. We will get

$$L(\dot{\xi}^I, \xi^I) = \hbar a_I \dot{\xi}^I - \dot{\theta}(\xi^I) - \bar{H}(\xi^I) = \hbar[a_I - \partial_I \theta]\dot{\xi}^I - \bar{H}(\xi^I)$$

  which gives rise to the same EOM.

  Change the phase space Lagrangian by a total time derivative of any function does not change the EOM.

Gauge "symmetry" and symmetry

Gauge redundancy (also called gauge symmetry by mistake) and **symmetry** (real physical symmetry) in quantum system:

- If we give a single quantum state two names $|a\rangle$ and $|b\rangle$, then $|a\rangle$ and $|b\rangle$ will have the same properties (since $|a\rangle = |b\rangle$). We say there is a gauge redundancy or gauge symmetry, and the theory of $|a\rangle$ and $|b\rangle$ is a gauge theory.
- If two orthogonal states $|a\rangle$ and $|b\rangle$ same properties, then we say there is a symmetry between $|a\rangle$ and $|b\rangle$ (since $\langle a|b\rangle = 0$).

Gauge "symmetry" is indeed a symmetry in classical system

Change of variables

- If we change the variables to $\eta^I = \eta^I(\xi^I)$, we get

$$L(\dot\eta^I, \eta^I) = \int \mathrm{d}t\ [\hbar a^\eta_I \dot\eta^I - \bar H(\eta^I)], \quad \hbar b^\eta_{IJ}\dot\eta^J = \frac{\partial \bar H}{\partial \eta^I},\ b^\eta_{IJ} = \partial_{\eta^I} a^\eta_J - \partial_{\eta^J} a^\eta_I$$

where

$$a^\eta_I = \mathrm{i}\langle\phi|\partial_{\eta^I}|\phi\rangle = \mathrm{i}\langle\phi|\partial_{\xi^J}|\phi\rangle \frac{\partial \xi^J}{\partial \eta^I} = a_J \frac{\partial \xi^J}{\partial \eta^I}.$$

$$\begin{aligned} b^\eta_{IJ} &= \partial_{\eta^I}(a_K \frac{\partial \xi^K}{\partial \eta^J}) - \partial_{\eta^J}(a_K \frac{\partial \xi^K}{\partial \eta^I}) = (\partial_{\eta^I} a_K)\frac{\partial \xi^K}{\partial \eta^J} - (\partial_{\eta^J} a_K)\frac{\partial \xi^K}{\partial \eta^I} \\ &= (\partial_{\xi^L} a_K)\frac{\partial \xi^L}{\partial \eta^I}\frac{\partial \xi^K}{\partial \eta^J} - (\partial_{\xi^L} a_K)\frac{\partial \xi^L}{\partial \eta^J}\frac{\partial \xi^K}{\partial \eta^I} = (\partial_{\xi^L} a_K - \partial_{\xi^K} a_L)\frac{\partial \xi^L}{\partial \eta^I}\frac{\partial \xi^K}{\partial \eta^J} \\ &= b_{LK}\frac{\partial \xi^L}{\partial \eta^I}\frac{\partial \xi^K}{\partial \eta^J} \end{aligned}$$

Generalized Liouville's theorm

- Consider time evolution from $t \to \tilde{t}$, $\xi^I \to \tilde{\xi}^I$. We have

$$\mathrm{d}^n \tilde{\xi}^I = \mathrm{Det}(\hat{J}) \mathrm{d}^n \xi^I, \quad J_{IJ} = \frac{\partial \tilde{\xi}^I}{\partial \xi^J}$$

For $\tilde{t} = t + \delta t$, $\tilde{\xi}^I = \xi^I + b^{IK} \frac{\partial \bar{H}}{\partial \xi^K} \delta t$, where $b_{IJ} b^{JK} = \delta_{IK}$.

$$J_{IJ} = \delta_{IJ} + \partial_J (b^{IK}) \frac{\partial \bar{H}}{\partial \xi^K} \delta t + b^{IK} \frac{\partial^2 \bar{H}}{\partial \xi^K \partial \xi^J} \delta t, \quad \mathrm{Det}(\hat{J}) = 1 + \partial_I (b^{IK}) \frac{\partial \bar{H}}{\partial \xi^K} \delta t$$

- Assume for η^I variable, b^η_{IJ} is indenpendent of η^I. Then (**Liouville's theorm**)

$$\mathrm{d}^n \eta^I = \mathrm{d}^n \tilde{\eta}^I, \quad \sqrt{\mathrm{Det}(b^\eta_{IJ})} \mathrm{d}^n \eta^I = \sqrt{\mathrm{Det}(\tilde{b}^\eta_{IJ})} \mathrm{d}^n \tilde{\eta}^I$$

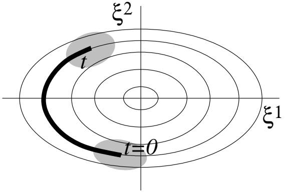
Change variables (**Generalized Liouville's theorem**)

$$\sqrt{\mathrm{Det}(b_{IJ})} \mathrm{Det}(\tfrac{\partial \xi^I}{\partial \eta^J})\ \mathrm{d}^n \xi^I \mathrm{Det}(\tfrac{\partial \eta^I}{\partial \xi^J}) = \sqrt{\mathrm{Det}(\tilde{b}^\eta_{IJ})} \mathrm{Det}(\tfrac{\partial \tilde{\xi}^I}{\partial \tilde{\eta}^J})\ \mathrm{d}^n \tilde{\eta}^I \mathrm{Det}(\tfrac{\partial \tilde{\eta}^I}{\partial \tilde{\xi}^J})$$

$$\sqrt{\mathrm{Det}(b_{IJ})} \mathrm{d}^n \xi^I = \sqrt{\mathrm{Det}(\tilde{b}_{IJ})} \mathrm{d}^n \tilde{\xi}^I \quad \text{or} \quad \mathrm{Pf}(b_{IJ}) \mathrm{d}^n \xi^I = \mathrm{Pf}(\tilde{b}_{IJ}) \mathrm{d}^n \tilde{\xi}^I$$

Phase space volume occupied by a quantum state

- For a classical theory every space-time point represents a distinct state. There is an ∞ number of states for a finite phase space.
- For a quantum system, $|\phi_{\xi^I(t)}\rangle$ and $|\phi_{\tilde{\xi}^I(t)}\rangle$ are orthogonal (*ie* are different quantum states) only when ξ^I and $\tilde{\xi}^I$ are different enough $\to$ uncertainty of ξ^I. There is a finite number of states for a finite phase space.



- A phase space region D^n contain how many quantum states? We guess

$$N = \int_{D^n} \frac{\mathrm{d}^n \xi^I}{(2\pi)^{n/2}} \mathrm{Pf}(b_{IJ})$$

We will confirm it later.

An example: an anharmonic oscillator

- What is low energy spectrum of (choose $\hbar = 1$ unit)

$$H = \frac{k^2}{2} + \frac{1}{2} v x^2 + \frac{1}{4} x^4, \quad k = -\mathrm{i}\partial_x$$

- Trial ground state:

$$|\psi_0\rangle = \left(\frac{\alpha}{\pi}\right)^{1/4} \mathrm{e}^{-\frac{1}{2}\alpha x^2}$$

The value of α is determined by minimizing the average energy

$$\langle \psi_0^\alpha | \hat{H} | \psi_0^\alpha \rangle = \frac{3 + 4\alpha^2 + 4\alpha v}{16\alpha^2}.$$

We find

$$\alpha = \frac{2 \times 6^{\frac{2}{3}}\, v + 6^{\frac{1}{3}} \left(27 + \sqrt{729 - 48\, v^3}\right)^{\frac{2}{3}}}{6 \left(27 + \sqrt{729 - 48\, v^3}\right)^{\frac{1}{3}}} = \sqrt{v} + \frac{3}{4v} + O(1/v^2)$$

$$\langle \hat{H} \rangle = \frac{1}{2}\sqrt{v} + \frac{3}{16v} + O(1/v^2)$$

An anharmonic oscillator

- Dynamical trial ground state

$$|\psi_{\xi^I}\rangle = \left(\frac{\alpha}{\pi}\right)^{1/4} \mathrm{e}^{\mathrm{i}\xi^2 x} \mathrm{e}^{-\frac{1}{2}\alpha(x-\xi^1)^2}$$

a state with position $x = \xi^1$ and momentum $k = \xi^2$ fluctuations.

$$L(\dot{\xi}^I, \xi^I) = \langle \psi_{\xi^I(t)} | \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} - H | \psi_{\xi^I(t)} \rangle = a_I(\xi^I)\dot{\xi}^I - \bar{H}(\xi^I)$$

where $a_I = \mathrm{i}\langle \psi_{\xi^I} | \frac{\partial}{\partial \xi^I} | \psi_{\xi^I} \rangle$, $\qquad \bar{H}(\xi^I) = \langle \psi_{\xi^I} | \hat{H} | \psi_{\xi^I} \rangle$

- The resulting equation of motion is given by

$$b_{IJ}\dot{\xi}^J = \frac{\partial \bar{H}}{\partial \xi^I}, \qquad b_{IJ} = \partial_I a_J - \partial_J a_I$$

- Calculate $a_I = \mathrm{i}\langle \psi_{\xi^I} | \frac{\partial}{\partial \xi^I} | \psi_{\xi^I} \rangle$:

$$a_1 = \mathrm{i} \int \mathrm{d}x \left(\frac{\alpha}{\pi}\right)^{1/2} \mathrm{e}^{-\mathrm{i}\xi^2 x} \mathrm{e}^{-\frac{1}{2}\alpha(x-\xi^1)^2} \alpha(x-\xi^1) \mathrm{e}^{\mathrm{i}\xi^2 x} \mathrm{e}^{-\frac{1}{2}\alpha(x-\xi^1)^2} = 0$$

$$a_2 = \mathrm{i} \int \mathrm{d}x \left(\frac{\alpha}{\pi}\right)^{1/2} \mathrm{e}^{-\mathrm{i}\xi^2 x} \mathrm{e}^{-\frac{1}{2}\alpha(x-\xi^1)^2} \mathrm{i}x \mathrm{e}^{\mathrm{i}\xi^2 x} \mathrm{e}^{-\frac{1}{2}\alpha(x-\xi^1)^2} = -\xi^1$$

An anharmonic oscillator

We find $b_{IJ} = -\epsilon_{ij}$ and

$$\bar{H}(\xi^I) = \frac{1}{2}(\xi^2)^2 + \frac{1}{2}v\Big(1+\frac{3}{2\alpha v}\Big)(\xi^1)^2 + \frac{1}{4}(\xi^1)^4 + \frac{3+4\,\alpha^3+4\,\alpha\, v}{16\,\alpha^2}$$

- The corresponding equation of motion has a form

$$\dot{\xi}^1 = \xi^2, \quad \dot{\xi}^2 = -v\Big(1+\frac{3}{2\alpha v}\Big)\xi^1 - (\xi^1)^3$$

- The number of quantum states

$$N = \int_{D^2} \frac{\mathrm{d}\xi^1\,\mathrm{d}\xi^2}{2\pi}\mathrm{Pf}(b_{IJ}) = \int_{D^2} \frac{\mathrm{d}\xi^1\,\mathrm{d}\xi^2}{2\pi} = \int_{D^2} \frac{\mathrm{d}x\,\mathrm{d}k}{2\pi}$$

which is what we expected.

An anharmonic oscillator

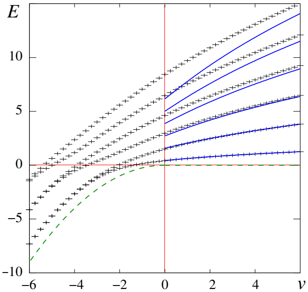
- The small motions around the ground state ξ_0^I $\to$ A collection of Harmonic oscillators $\to$ low energy spectrum.

- This is why for many interacting systems, the low energy excitations are non-interacting (like phonons in interacting crystals).
- This is why semi-classical approach works well for many systems.

- For small motion around the ground state $\xi^1 = 0, \xi^2 = 0$:

$$\dot{\xi}^1 = \xi^2, \quad \dot{\xi}^2 = -v\Big(1 + \frac{3}{2\alpha v}\Big)\xi^1$$

A harmonic oscillator with mass $m = 1$, spring constant $K = \frac{3\alpha+2\alpha^2 v}{2\alpha^2}$, and frequency $\omega = \sqrt{v(1 + \frac{3}{2\alpha v})}$.



- Re-quantizing the harmonic oscillator $\to$ low energy spectrum for the Hamiltonian

$$H = \frac{k^2}{2} + \frac{1}{2}vx^2 + \frac{1}{4}x^4, \qquad k = -\mathrm{i}\partial_x$$

$a_I = \mathrm{i}\langle\psi_{\xi^I}|\frac{\partial}{\partial\xi^I}|\psi_{\xi^I}\rangle$ is the so call **geometric phase** (Berry Phase).

- *What is the geometric phase?*
  Consider $|\psi_{\xi^I}\rangle$ and $|\psi_{\xi^I+\delta\xi^I}\rangle$, what is the phase different between $|\psi_{\xi^I}\rangle$ and $|\psi_{\xi^I+\delta\xi^I}\rangle$?
- But $|\psi_{\xi^I}\rangle$ and $|\psi_{\xi^I+\delta\xi^I}\rangle$ are not parallel: $|\psi_{\xi^I+\delta\xi^I}\rangle \neq \mathrm{e}^{\mathrm{i}\delta\phi}|\psi_{\xi^I}\rangle$.
  They differ by more than a phase.
- But for small $\delta\xi^I$

$$\langle\psi_{\xi^I}|\psi_{\xi^I+\delta\xi^I}\rangle \approx 1 + \mathrm{i}\,O(\delta\xi^I), \qquad \langle\psi_{\xi^I+\delta\xi^I}|\psi_{\xi^I}\rangle \approx 1 - \mathrm{i}\,O(\delta\xi^I)$$

since, to the first order in δ

$$0 = \delta\langle\psi_{\xi^I}|\psi_{\xi^I}\rangle = (\langle\psi_{\xi^I+\delta\xi^I}| - \langle\psi_{\xi^I}|)|\psi_{\xi^I}\rangle + \langle\psi_{\xi^I}|(|\psi_{\xi^I+\delta\xi^I}\rangle - |\psi_{\xi^I}\rangle)$$
$$= [\langle\psi_{\xi^I+\delta\xi^I}|\psi_{\xi^I}\rangle - 1] + [\langle\psi_{\xi^I}|\psi_{\xi^I+\delta\xi^I}\rangle - 1]$$

Therefore $\langle\psi_{\xi^I}|\psi_{\xi^I+\delta\xi^I}\rangle \approx \mathrm{e}^{\mathrm{i}\,O(\delta\xi)}$, or

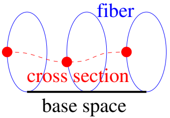
$$|\psi_{\xi^I+\delta\xi^I}\rangle = \mathrm{e}^{\mathrm{i}\delta\phi}|\psi_{\xi^I}\rangle + \#(\delta\xi^I)^2, \qquad \delta\phi = a_I(\xi^I)\delta\xi^I$$

$U(1)$ fiber bundle and global view of geometric phase

The physical states are characterized by a point ξ^i on the phase-space, after we pick the phase of $|\psi(\xi^i)\rangle$. Different choices of phases are equivalent $\to$ the notion of $U(1)$ fiber bundle:

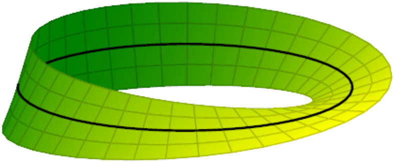
- The phase space ξ^i is the base space. The equivalent normalized quantum states $e^{i\phi}|\psi(\xi^i)\rangle$ form the fiber, which is S^1.

- So, a $U(1)$ fiber bundle is (locally) $S^1 \times$ phase-space.
- the ξ^i-labeled quantum states $|\psi(\xi^i)\rangle$ is a cross section of the $U(1)$ bundle. **Pick a phase = pick a cross section.**



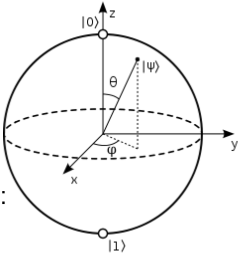
- Trivial $U(1)$ bundle $= S^1 \times$ base-space (globally).
- Non-trivial $U(1)$ fiber bundle different topology from $S^1 \times$ base-space. No smooth cross section. $\to$ A different class of classical system.

- **An example**: Möbius strip is a non-trivial I bundle on base-space S^1 ($I = [0, 1]$ is the fiber)

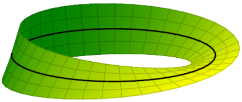


Spin-1/2 example: geometric phase and fiber bundle

- All possible spin-1/2 states (or qubit states)
  $$(a+\mathrm{i}b)|\uparrow\rangle + (c+\mathrm{i}d)|\downarrow\rangle = \begin{pmatrix} a+\mathrm{i}b \\ c+\mathrm{i}d \end{pmatrix} = z,\ \ a^2+b^2+c^2+d^2=1$$
  form a 3-dimensional sphere S^3 (a sphere in 4-dimensional space).
- But since $|\psi\rangle \sim \mathrm{e}^{\mathrm{i}\phi}|\psi\rangle$, all possible spin-1/2 states (or qubit states) actually form a 2-dimensional sphere S^2. $z^\dagger \boldsymbol{\sigma} z = \boldsymbol{n}$: a map $S^3 \to S^2 \to |\boldsymbol{n}\rangle$: spin-1/2 in $\boldsymbol{n}$ direction.



- S^3 locally looks like $S^1 \times S^2$: S^3 is a **fiber bundle** with **fiber** S^1 and **base space** S^2:
  $$pt \to S^1 \xrightarrow{inj} S^3 \xrightarrow{surj} S^2 \to pt$$
- If we pick a phase ϕ for each $|\boldsymbol{n}\rangle$,
  we may get $|\boldsymbol{n}\rangle = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\varphi/2}\cos(\theta/2) \\ \mathrm{e}^{\mathrm{i}\varphi/2}\sin(\theta/2) \end{pmatrix}$
  or $|\boldsymbol{n}\rangle = \begin{pmatrix} \cos(\theta/2) \\ \mathrm{e}^{\mathrm{i}\varphi}\sin(\theta/2) \end{pmatrix}$



Möbius strip locally $I \times S^1$

- The above correspond to two cross sections of the fiber bundle.

What is the geometric phase?

In the above, the phase ϕ for each $|\boldsymbol{n}\rangle$ is chosen quite arbitarily. Can we make better choice?

- Let us compare the phase of $|\boldsymbol{n}(\theta,\varphi)\rangle$ and $|\boldsymbol{n}(\theta+\delta\theta,\varphi+\delta\varphi)\rangle$:

$$
\begin{aligned}
&\langle \boldsymbol{n}(\theta,\varphi)|\boldsymbol{n}(\theta+\delta\theta,\varphi+\delta\varphi)\rangle \\
&= 1 + \underbrace{\langle \boldsymbol{n}(\theta,\varphi)|\frac{\partial}{\partial\theta}|\boldsymbol{n}(\theta,\varphi)\rangle}_{\mathrm{i}\, a_\theta}\delta\theta + \underbrace{\langle \boldsymbol{n}(\theta,\varphi)|\frac{\partial}{\partial\varphi}|\boldsymbol{n}(\theta,\varphi)\rangle}_{\mathrm{i}\, a_\varphi}\delta\varphi \\
&= 1 + \mathrm{i}\, a_\theta\delta\theta + \mathrm{i}\, a_\varphi\delta\varphi \approx \mathrm{e}^{\mathrm{i}\,(a_\theta\delta\theta + a_\varphi\delta\varphi)},
\end{aligned}
$$

where $\mathrm{i}\, a_\theta = \langle \boldsymbol{n}(\theta,\varphi)|\frac{\partial}{\partial\theta}|\boldsymbol{n}(\theta,\varphi)\rangle$ and $\mathrm{i}\, a_\varphi = \langle \boldsymbol{n}(\theta,\varphi)|\frac{\partial}{\partial\varphi}|\boldsymbol{n}(\theta,\varphi)\rangle$

- $\mathrm{e}^{\mathrm{i}\,(a_\theta\delta\theta + a_\varphi\delta\varphi)} = \mathrm{e}^{\mathrm{i}\,\boldsymbol{a}\cdot\Delta\boldsymbol{n}}$ is the **geometric phase** as we change $|\boldsymbol{n}(\theta,\varphi)\rangle$ to $|\boldsymbol{n}(\theta+\delta\theta,\varphi+\delta\varphi)\rangle = |\boldsymbol{n}+\Delta\boldsymbol{n}\rangle$.
- $\boldsymbol{a} = (a_\theta, a_\varphi)$ is the **connection (vector potential)** of the geometric phase. (Like the vector potential in electromagnetism.)

Is the geometric phase meaningless?

- If $\langle \boldsymbol{n}|\boldsymbol{n}+\Delta\boldsymbol{n}\rangle = \mathrm{e}^{\mathrm{i}\boldsymbol{a}\cdot\Delta\boldsymbol{n}}$, we can always change the phase of $|\boldsymbol{n}+\Delta\boldsymbol{n}\rangle \to |\boldsymbol{n}+\Delta\boldsymbol{n}\rangle_1 = \mathrm{e}^{-\mathrm{i}\boldsymbol{a}\cdot\Delta\boldsymbol{n}}|\boldsymbol{n}+\Delta\boldsymbol{n}\rangle$, so that $\langle \boldsymbol{n}|\boldsymbol{n}+\Delta\boldsymbol{n}\rangle_1 = \mathrm{e}^{-\mathrm{i}\boldsymbol{a}\cdot\Delta\boldsymbol{n}}\mathrm{e}^{\mathrm{i}\boldsymbol{a}\cdot\Delta\boldsymbol{n}} = 1$.
  We can always make geometric phase = 0, and the geometric phase is meaningless. Wrong!
- As we change the phase of $|\boldsymbol{n}\rangle$: $|\boldsymbol{n}\rangle \to \mathrm{e}^{\mathrm{i}f(\theta,\varphi)}|\boldsymbol{n}\rangle$, the geometric phase (*ie* the connection) also changes:

$$(a_\theta, a_\varphi) \to (a_\theta + \partial_\theta f, a_\varphi + \partial_\varphi f)$$

- We can always choose a f to make $(a_\theta, a_\varphi) = (0,0)$ at any chosen (θ, φ), *ie* to make $|\boldsymbol{n}\rangle$ and $|\boldsymbol{n}+\Delta\boldsymbol{n}\rangle$ to have the same phase.
- But since $S^3 \to S^2$ is not a trivial bundle, we cannot find a f to make $(a_\theta, a_\varphi) = (0,0)$ for all (θ, φ), *ie* to make all $|\boldsymbol{n}\rangle$'s to have the same phase. There is no crossection such that $|\boldsymbol{n}\rangle$ all have the same phases (*ie* $(a_\theta, a_\varphi) = (0,0)$ for all (θ, φ)).

Some part of the geometric connection $\boldsymbol{a} = (a_\theta, a_\varphi)$ is physical, and other part is not.

The notion of the "flux" of the geometric phase

- Consider a loop $|\boldsymbol{n}(t)\rangle$, $t \in [0,1]$, $\boldsymbol{n}(0) = \boldsymbol{n}(1)$. The total geometric phase of the loop
$$\mathrm{e}^{\mathrm{i}\sum \delta\varphi(t)} = \langle \boldsymbol{n}(0)|\boldsymbol{n}(t_1)\rangle\langle \boldsymbol{n}(t_1)|\boldsymbol{n}(t_2)\rangle\langle \boldsymbol{n}(t_2)|\boldsymbol{n}(t_3)\rangle \cdots \langle \boldsymbol{n}(t_{N-1})|\boldsymbol{n}(1)\rangle$$
$$= \mathrm{e}^{\mathrm{i}\sum \boldsymbol{a}(t)\cdot\delta\boldsymbol{n}(t)} = \mathrm{e}^{\mathrm{i}\int \boldsymbol{a}(t)\cdot \mathrm{d}\boldsymbol{n}(t)} = \mathrm{e}^{\mathrm{i}\int \boldsymbol{a}(t)\cdot\frac{\mathrm{d}\boldsymbol{n}(t)}{\mathrm{d}t}\mathrm{d}t}$$
- If we change the phase of $|\boldsymbol{n}\rangle$: $|\boldsymbol{n}\rangle \to \mathrm{e}^{\mathrm{i}f(\boldsymbol{n})}|\boldsymbol{n}\rangle$, the total geometric phase for a loop – the **geometric flux** – does not change.
- Computing the geometric flux:
$$\oint_C \boldsymbol{a}\cdot \mathrm{d}\boldsymbol{n} = \oint_C a_\theta \mathrm{d}\theta + a_\varphi \mathrm{d}\varphi = \iint_D (\partial_\theta a_\varphi - \partial_\varphi a_\theta)\mathrm{d}\theta\,\mathrm{d}\varphi$$
where $C = \partial D$, *ie* the loop C is the boundary of the disk D.

\- $b = \partial_\theta a_\varphi - \partial_\varphi a_\theta$ is called the geometric curvature (magnetic field): $b\Delta\theta\Delta\varphi =$ the total geometric phase for a small loop $(\theta,\varphi) \to (\theta+\Delta\theta,\varphi) \to (\theta+\Delta\theta,\varphi+\Delta\varphi) \to (\theta\theta,\varphi+\Delta\varphi) \to (\theta,\varphi)$.

- The total geometric phase for a loop $\oint_C \boldsymbol{a}\cdot\mathrm{d}\boldsymbol{n}$ and the geometric curvature b are meaningful, since they are invariant under the **gauge transformation** $|\boldsymbol{n}\rangle \to \mathrm{e}^{\mathrm{i}f(\boldsymbol{n})}|\boldsymbol{n}\rangle$ and $\boldsymbol{a} \to \boldsymbol{a} + \partial f$.

The geometric phase (the flux) for spin-1/2

From $\mathrm{i}\, a_\theta = \langle \boldsymbol{n}(\theta,\varphi)|\frac{\partial}{\partial\theta}|\boldsymbol{n}(\theta,\varphi)\rangle$ and $\mathrm{i}\, a_\varphi = \langle \boldsymbol{n}(\theta,\varphi)|\frac{\partial}{\partial\varphi}|\boldsymbol{n}(\theta,\varphi)\rangle$ and $|\boldsymbol{n}\rangle = \begin{pmatrix} \cos(\theta/2) \\ \mathrm{e}^{\mathrm{i}\varphi}\sin(\theta/2) \end{pmatrix}$, we find that

$$a_\theta = 0, \qquad a_\varphi = \sin(\theta/2)\sin(\theta/2) = \frac{1-\cos(\theta)}{2}$$

"Flux" of geometric phase: total geometric phase around a loop

For a loop $(\theta,\varphi) \to (\theta+\Delta\theta,\varphi) \to (\theta+\Delta\theta,\varphi+\Delta\varphi) \to (\theta\theta,\varphi+\Delta\varphi) \to (\theta,\varphi)$:

$$\oint_{[\Delta\theta,\Delta\varphi]} a_\theta\, \mathrm{d}\theta + a_\varphi\, \mathrm{d}\varphi = 0 + \frac{1-\cos(\theta+\Delta\theta)}{2}\Delta\varphi + 0 - \frac{1-\cos(\theta)}{2}\Delta\varphi$$

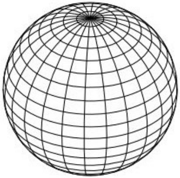
$$= \frac{1}{2}\sin(\theta)\Delta\theta\Delta\varphi = \frac{1}{2}\Omega([\Delta\theta,\Delta\varphi]) \quad \to \quad \text{half of the solid angle.}$$

- The total "flux" of the geometric phase on any campact space S^2 must be quantized

$$\int_{C^2} \frac{1}{2!} b_{IJ}\, \mathrm{d}\xi^I\, \mathrm{d}\xi^J = 2\pi \times \text{integer}$$

$$= 2\pi \times \text{Chern number.}$$

Spin-1/2 has a Chern number 1



The geometric phase of spin-1

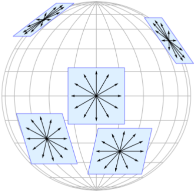
- The geometric connection for spin-1/2 $|\boldsymbol{n}_{S_{\boldsymbol{n}}=\frac{1}{2}}\rangle$ is $(a_\theta^{S=\frac{1}{2}}, a_\varphi^{S=\frac{1}{2}}) = (0, \frac{1-\cos(\theta)}{2})$.
- The geometric connection for spin-1 $|\boldsymbol{n}_{S_{\boldsymbol{n}}=1}\rangle$ is $(a_\theta^{S=1}, a_\varphi^{S=1}) = 2(a_\theta^{S=\frac{1}{2}}, a_\varphi^{S=\frac{1}{2}}) = (0, 1-\cos(\theta))$.

\- This is because we may view $|\boldsymbol{n}_{S_{\boldsymbol{n}}=1}\rangle = |\boldsymbol{n}_{S_{\boldsymbol{n}}=\frac{1}{2}}\rangle \otimes |\boldsymbol{n}_{S_{\boldsymbol{n}}=\frac{1}{2}}\rangle$

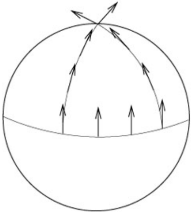
$$\mathrm{e}^{\mathrm{i}\Delta\phi^{S=1}} = \langle \boldsymbol{n}_{S_{\boldsymbol{n}}=1}|\boldsymbol{n}'_{S_{\boldsymbol{n}}=1}\rangle = \langle \boldsymbol{n}_{S_{\boldsymbol{n}}=\frac{1}{2}}|\boldsymbol{n}'_{S_{\boldsymbol{n}}=\frac{1}{2}}\rangle \times \langle \boldsymbol{n}_{S_{\boldsymbol{n}}=\frac{1}{2}}|\boldsymbol{n}'_{S_{\boldsymbol{n}}=\frac{1}{2}}\rangle = \mathrm{e}^{\mathrm{i}2\Delta\phi^{S=\frac{1}{2}}}$$

How to visualize the geometric phase of spin-1

Different arrows in the plan at a point $\boldsymbol{n}$ on the sphere correspond to the different phase choices $\mathrm{e}^{\mathrm{i}\phi}|\boldsymbol{n}_{S_{\boldsymbol{n}}=1}\rangle$. We try to choose ϕ for the spin-1 states along the loop, such that $|\boldsymbol{n}_{S_{\boldsymbol{n}}=1}\rangle$ all have the same phase. But after going around the loop, the phase miss match is the total geometric phase along the loop.

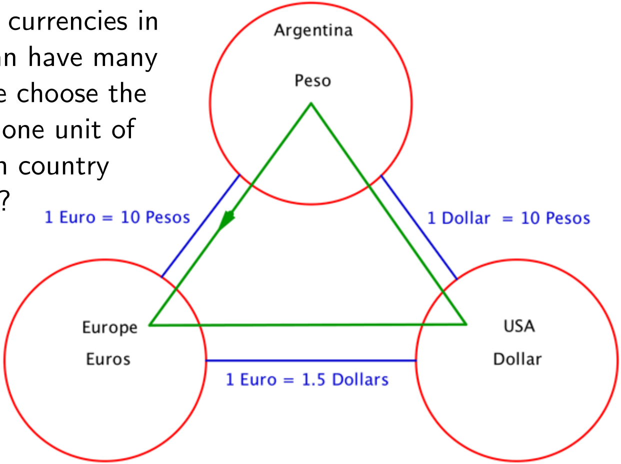


Tangent bundle on a 2-sphere



The geometric phase and currency exchange

- The phase of the state $|\boldsymbol{n}\rangle$ for a spin in $\boldsymbol{n}$ direction can have many choices. Can we choose a phase for each $|\boldsymbol{n}\rangle$ such that all the states $|\boldsymbol{n}\rangle$ have a same phase? *Only when* $b_{IJ} = 0$.
- The unit of the currencies in each country can have many choices. Can we choose the units such that one unit of currency in each country worth the same?



Why do we care about such a subtle geometric phase?

The geometric phase is a quantum effect that can affect the equation of motion. Its effect can be real and not subtle in quantum materials.

Classical motion of spin-1/2: two views

The phase-space action

$$S = \int \mathrm{d}t[\frac{1}{2}(1-\cos\theta)\dot\varphi - V(\theta,\varphi)] = \int \mathrm{d}t[-\frac{1}{2}\cos\theta\dot\varphi - V(\theta,\varphi)] + ...$$

- Near the equator, $\cos\theta = \frac{\pi}{2} - \theta = L_z$:
$$S = \int \mathrm{d}t[L_z\dot\varphi - V(\frac{\pi}{2} - L_z, \varphi)]$$

- The uniform phase-space magnetic field $\to$ the usual canonical coordinate-momentum pair.

- $L = p\dot x - H(p,x)$ $\to$ uniform phase-space magnetic field $a_p = 0, a_x = p$ and $b_{px} = \partial_p a_x - \partial_x a_p = 1$.

- A particle moving on S^2 with a uniform magnetic field $b_{\theta\varphi}$ of total flux 2π. It is the motion in the lowest Landau level assuming $\hbar\omega_c$ is large. Modified Newton law $\boldsymbol{F} = \boldsymbol{v}\times\boldsymbol{B}$ (not $\boldsymbol{F} = m\boldsymbol{a}$).

- A sphere with a uniform magnetic field of $2\pi N_{\text{Chern}}$ flux $\to$ lowest Landau level has $N_{\text{Chern}}+1$-fold degeneracy $\to$ spin-$N_{\text{Chern}}/2$.

The motion of a neutron in a non-uniform magnetic field

Consider a spin-1/2 neutron moving in a strong non-uniform **spin magnetic field** $\boldsymbol{B}(\boldsymbol{x})$. The neutron magnetic moment is $\mu_n = -1.91304272(45)\mu_N$, where $\mu_N = \frac{e\hbar}{2m_p}$ in SI unit (or $\mu_N = \frac{e\hbar}{2m_p c}$ in CGS unit). The interaction between the magnetic moment and the magnetic field, $-\mu_n \boldsymbol{B}\cdot\boldsymbol{\sigma}$, will force the neutron spin to be anti-parallel to the magnetic field $\boldsymbol{B}$ at low energies.

- *What is the quantum Hamiltonian $\hat{H}$ that describes the quantum motion of the above low energy neutron?*
- *What is the classical equation that describes the motion of the above low energy neutron?*

Our first guess:

- $\hat{H} = -\frac{\hbar^2}{2m_n}\boldsymbol{\partial}^2 + V(\boldsymbol{x})$ where $V(\boldsymbol{x}) = -|\mu_n \boldsymbol{B}(\boldsymbol{x})|$ is the effective potential energy.

Is this guess correct?

Schrödinger equation and coordinate basis

- Schrödinger equation (basis independent): $\mathrm{i}\hbar\partial_t|\psi\rangle = \hat{H}(\hat{\boldsymbol{p}}, \hat{\boldsymbol{x}})|\psi\rangle$
- In a coordinate basis $|\psi\rangle = \int \mathrm{d}\boldsymbol{x}\ \psi(\boldsymbol{x})|\boldsymbol{x}\rangle$, it becomes

$$\mathrm{i}\hbar\partial_t\psi(\boldsymbol{x},t) = H(\frac{1}{\mathrm{i}\hbar}\boldsymbol{\partial}, \boldsymbol{x})\psi(\boldsymbol{x},t) = \Big(-\frac{\hbar^2}{2m_n}\boldsymbol{\partial}^2 + V(\boldsymbol{x})\Big)\psi(\boldsymbol{x},t)$$

- In the above, we have assumed that there is no geometric phase for $|\boldsymbol{x}\rangle$,*ie* the phase change from $|\boldsymbol{x}\rangle$ to $|\boldsymbol{x}+\delta\boldsymbol{x}\rangle$ is 0.
- But for our neutron problem, the phase from $|\boldsymbol{x}\rangle$ to $|\boldsymbol{x}+\delta\boldsymbol{x}\rangle$ is not 0. *How to to compute the phase change?*

- For our neutron problem, $|\boldsymbol{x}\rangle$ is actually $|\boldsymbol{x}\rangle\otimes|\boldsymbol{n}(\boldsymbol{x})\rangle$.
- The phase change from $|\boldsymbol{x}\rangle\otimes|\boldsymbol{n}(\boldsymbol{x})\rangle$ to $|\boldsymbol{x}+\delta\boldsymbol{x}\rangle\otimes|\boldsymbol{n}(\boldsymbol{x}+\delta\boldsymbol{x})\rangle$ is given by $\boldsymbol{a}\cdot\delta\boldsymbol{x}$:

$$\mathrm{e}^{\mathrm{i}\,\boldsymbol{a}(\boldsymbol{x})\cdot\delta\boldsymbol{x}} = \langle\boldsymbol{n}(\boldsymbol{x})|\boldsymbol{n}(\boldsymbol{x}+\delta\boldsymbol{x})\rangle \quad\to\quad \mathrm{i}\,\boldsymbol{a}(\boldsymbol{x}) = \langle\boldsymbol{n}(\boldsymbol{x})|\boldsymbol{\partial}|\boldsymbol{n}(\boldsymbol{x})\rangle$$

- *If there is a geometric phase for $|\boldsymbol{x}\rangle$, ie a phase change $\mathrm{e}^{\mathrm{i}\,\boldsymbol{a}(\boldsymbol{x})\cdot\delta\boldsymbol{x}}$ from $|\boldsymbol{x}\rangle$ to $|\boldsymbol{x}+\delta\boldsymbol{x}\rangle$, what will the Schrödinger equation look like?*

- The result $\hat{H} = -\frac{\hbar^2}{2m_n}\boldsymbol{\partial}^2 - |\mu_n\boldsymbol{B}(\boldsymbol{x})|$ is valid only if the direction of $\boldsymbol{B}(\boldsymbol{x})$ does not change.

How geometric phase affects Schrödinger equation?

- If we choose a new basis $|\boldsymbol{x}\rangle_{\text{tw}} = \mathrm{e}^{\mathrm{i}\phi(\boldsymbol{x})}|\boldsymbol{x}\rangle$. $|\boldsymbol{x}\rangle_{\text{tw}}$ will have an non-zero geometric phase: The phase change from $|\boldsymbol{x}\rangle_{\text{tw}}$ to $|\boldsymbol{x}+\delta\boldsymbol{x}\rangle_{\text{tw}}$ is $\mathrm{e}^{\mathrm{i}[\phi(\boldsymbol{x}+\delta\boldsymbol{x})-\phi(\boldsymbol{x})]} = \mathrm{e}^{\mathrm{i}\,\boldsymbol{a}(\boldsymbol{x})\cdot\delta\boldsymbol{x}}$ where $\boldsymbol{a} = \boldsymbol{\partial}\phi(\boldsymbol{x})$.
- What is the Schrödinger equation in the new basis $|\psi\rangle = \int \mathrm{d}\boldsymbol{x}\ \psi(\boldsymbol{x})|\boldsymbol{x}\rangle = \int \mathrm{d}\boldsymbol{x}\ \psi_{\text{tw}}(\boldsymbol{x})|\boldsymbol{x}\rangle_{\text{tw}}$ or $\mathrm{e}^{\mathrm{i}\phi(\boldsymbol{x})}\psi_{\text{tw}} = \psi(\boldsymbol{x})$

$$\mathrm{i}\hbar\partial_t\psi(\boldsymbol{x},t) = \hat{H}\psi(\boldsymbol{x},t) = \hat{H}\mathrm{e}^{\mathrm{i}\phi(\boldsymbol{x})}\psi_{\text{tw}}$$
$$\mathrm{e}^{-\mathrm{i}\phi(\boldsymbol{x})}\mathrm{i}\hbar\partial_t\psi(\boldsymbol{x},t) = \mathrm{e}^{-\mathrm{i}\phi(\boldsymbol{x})}\hat{H}\mathrm{e}^{\mathrm{i}\phi(\boldsymbol{x})}\psi_{\text{tw}}$$
$$\mathrm{i}\hbar\partial_t\psi_{\text{tw}}(\boldsymbol{x},t) = \hat{H}_{\text{tw}}\psi_{\text{tw}}, \qquad \hat{H}_{\text{tw}} = \mathrm{e}^{-\mathrm{i}\phi(\boldsymbol{x})}\hat{H}\mathrm{e}^{\mathrm{i}\phi(\boldsymbol{x})}.$$

- $\hat{H}_{\text{tw}}(\boldsymbol{\partial},\boldsymbol{x})$ is obtained from $\hat{H}(\boldsymbol{\partial},\boldsymbol{x})$ by replacing $\boldsymbol{\partial}$ in $\hat{H}$ by $\mathrm{e}^{-\mathrm{i}\phi(\boldsymbol{x})}\boldsymbol{\partial}\mathrm{e}^{\mathrm{i}\phi(\boldsymbol{x})} = \boldsymbol{\partial} + \mathrm{i}\boldsymbol{\partial}\phi(\boldsymbol{x}) = \boldsymbol{\partial} + \mathrm{i}\boldsymbol{a}(\boldsymbol{x})$.

$$\hat{H}_{\text{tw}} = \hat{H}(\boldsymbol{\partial}+\mathrm{i}\boldsymbol{a},\boldsymbol{x}) = -\frac{\hbar^2}{2m_n}(\boldsymbol{\partial}+\mathrm{i}\boldsymbol{a})^2 + V.$$

The above is how geometric phase affects Schrödinger equation.

Effective Hamiltonian for neutron in spin magnetic field

$$\hat{H}_{\text{eff}} = -\frac{\hbar^2}{2m_n}(\boldsymbol{\partial} + \mathrm{i}\boldsymbol{a})^2 + V$$

where

$$\mathrm{i}\boldsymbol{a}(\boldsymbol{x}) = \langle \boldsymbol{n}(\boldsymbol{x})|\partial|\boldsymbol{n}(\boldsymbol{x})\rangle, \quad \boldsymbol{n} = -\frac{\boldsymbol{B}(\boldsymbol{x})}{|\boldsymbol{B}(\boldsymbol{x})|}, \quad V(\boldsymbol{x}) = -|\mu_n \boldsymbol{B}(\boldsymbol{x})|.$$

$\boldsymbol{a}(\boldsymbol{x})$ comes from geometric phase and $V(\boldsymbol{x})$ is potential energy.

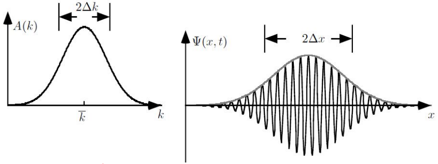
- $V(\boldsymbol{x})$ generates a potential force $\boldsymbol{F} = -\boldsymbol{\partial} V$ on the particle.

- We will see that $\boldsymbol{a}(\boldsymbol{x})$ *generates a Lorentz force* $\boldsymbol{F} \propto \boldsymbol{v} \times \boldsymbol{b}$ *on the particle, as if there is a "orbital magnetic field"* $\boldsymbol{b} = \boldsymbol{\partial} \times \boldsymbol{a}$.

The geometric phase gives rise to an effective orbital magnetic field.

Obtain classical equation of motion

- Consider wavepacket with space-time dependent spin



$$|\psi_{\boldsymbol{x}_0,\boldsymbol{k}_0}\rangle = \left(\frac{\alpha}{\pi}\right)^{1/4} \mathrm{e}^{\mathrm{i}\,\boldsymbol{k}_0\boldsymbol{x}}\, \mathrm{e}^{-\frac{1}{2}\alpha(\boldsymbol{x}-\boldsymbol{x}_0)^2} |\boldsymbol{n}(\boldsymbol{x}_0)\rangle$$

Phase space Lagrangian

$$\mathcal{L} = \langle\psi_{\boldsymbol{x}_0(t),\boldsymbol{k}_0(t)}|\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t} - H|\psi_{\boldsymbol{x}_0(t),\boldsymbol{k}_0(t)}\rangle$$

$$= \hbar\underbrace{\boldsymbol{a}'}_{=0}\cdot\dot{\boldsymbol{x}}_0 + \hbar\underbrace{\boldsymbol{a}''}_{-\boldsymbol{x}_0}\cdot\dot{\boldsymbol{k}}_0 + \hbar\underbrace{\boldsymbol{a}(\boldsymbol{x}_0)}_{-\mathrm{i}\,\langle\boldsymbol{n}|\partial_{\boldsymbol{x}_0}|\boldsymbol{n}\rangle}\cdot\dot{\boldsymbol{x}}_0 - \frac{\hbar^2\boldsymbol{k}_0^2}{2m_n} - |\mu_n\boldsymbol{B}(\boldsymbol{x}_0)|$$

$$= -\hbar\boldsymbol{x}_0\cdot\dot{\boldsymbol{k}}_0 + \hbar\boldsymbol{a}(\boldsymbol{x}_0)\cdot\dot{\boldsymbol{x}}_0 - \frac{\hbar^2\boldsymbol{k}_0^2}{2m_n} + |\mu_n\boldsymbol{B}(\boldsymbol{x}_0)|$$

$$\approx \boldsymbol{p}_0\cdot\dot{\boldsymbol{x}}_0 + \hbar\boldsymbol{a}(\boldsymbol{x}_0)\cdot\dot{\boldsymbol{x}}_0 - \frac{\boldsymbol{p}_0^2}{2m_n} - V(\boldsymbol{x}_0)$$

Obtain classical equation of motion

For $S = \int \mathrm{d}t\ [\boldsymbol{p} \cdot \dot{\boldsymbol{x}} + \hbar \boldsymbol{a}(\boldsymbol{x}) \cdot \dot{\boldsymbol{x}} - \frac{\boldsymbol{p}^2}{2m_n} - V(\boldsymbol{x})]$

From $\int \mathrm{d}t\ \hbar\delta(a_i(\boldsymbol{x})\dot{x}^i) = \int \mathrm{d}t\ \hbar[\delta x^j(\partial_j a_i)\dot{x}^i - \dot{a}_i(\boldsymbol{x})\delta x^i]$

$$\delta S = \int \mathrm{d}t\ \delta p_i[\dot{x}^i - \frac{p_i}{m_n}] + \delta x^i[-\dot{p}_i + \hbar(\partial_i a_J)\dot{x}^j - \hbar(\partial_j a_i)\dot{x}^j - \partial_i V]$$

we obtain the phase space equation of motion

$$\dot{x}^i = \frac{p_i}{m_n}, \qquad \dot{p}_i = \underbrace{\hbar(\partial_i a_J - \partial_j a_i)\dot{x}^j}_{\text{Lorentz force}} - \partial_i V = \hbar b_{IJ}\dot{x}^j - \partial_i V$$

Spin twist gives rise to simulated vector potential
$\boldsymbol{a}(\boldsymbol{x}) = -\mathrm{i}\langle \boldsymbol{n}(\boldsymbol{x})|\partial|\boldsymbol{n}(\boldsymbol{x})\rangle \to$ **simulated magnetic field.**

Geometric phase = orbital magnetic field

- Equation of motion for $x^3 = z$

$$m_n \ddot{z} = -\partial_z V + \dot{x}[\partial_z \hbar a_x - \partial_x \hbar a_z] + \dot{y}[\partial_z \hbar a_y - \partial_y \hbar a_z]$$

- Compare with the equation of motion in a magnetic field $\boldsymbol{B}$

$$\begin{aligned} m_n \ddot{z} &= -\partial_z V + \frac{e}{c}(\dot{x} B_y - \dot{y} B_x) \\ &= -\partial_z V + \dot{x}(\partial_z \frac{e}{c} A_x - \partial_x \frac{e}{c} A_z) - \dot{y}(\partial_y \frac{e}{c} A_z - \partial_z \frac{e}{c} A_y). \end{aligned}$$

- We find that $\hbar \boldsymbol{a} = \frac{e}{c} \boldsymbol{A}$

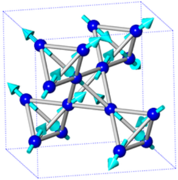
- **The geometric meaning of magnetic field**

$$\# \text{ of flux quanta} = \int_S \mathrm{d}\boldsymbol{S} \cdot \boldsymbol{B} \Big/ \frac{hc}{e} = \oint_{\partial S} \mathrm{d}\boldsymbol{x} \cdot \frac{e}{hc} \boldsymbol{A} = \frac{1}{2\pi} \oint_{\partial S} \mathrm{d}\boldsymbol{x} \cdot \boldsymbol{a}$$
$$= \text{geometric phase around a loop}/2\pi$$

Simulate orbital magnetic field by twisted spin

When an electron move in a background twisted spins, the electron spin may following the direction of the background twisted spins $\to$ geometric phase = simulated magnetic field.

The geometric phase around a loop/2π = The number of flux quanta of the simulated magnetic field through the loop.



- Note that $hc/e = 4.135667516 \times 10^{-15}\text{T m}^2$.

- If there is one flux quantum per $(10^{-8}m)^2$, then $B = 4.135667516 \times 10^{-15}/(10^{-8})^2 = 41\text{T}$ (About the highest static magnetic field produced)

- For electron hoping in a non-coplannar magnet, the geometric phase from the spin-twist is of order 1 per unit cell: There is one flux quantum per $(10^{-9}m)^2$, or the simulated magnetic field by the spin-twist geometric phase is $B_{\text{spin}} = 4.135667516 \times 10^{-15}/(10^{-9})^2 = 4100\text{T}$

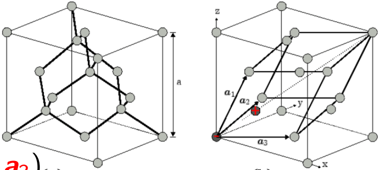
Energy bands in a crystal

- Hopping Hamiltonian

$$H_{\boldsymbol{m}\alpha;\boldsymbol{n}\beta} = \sum_{\Delta\boldsymbol{n}} -t^{\Delta\boldsymbol{n}}_{\alpha\beta}\delta_{\boldsymbol{m},\boldsymbol{n}+\Delta\boldsymbol{n}},$$

  $\boldsymbol{n}$ lable unit cell, α, β label orbitals

Si



(a) (b)

- Plane wave state ($\boldsymbol{x_n} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$)

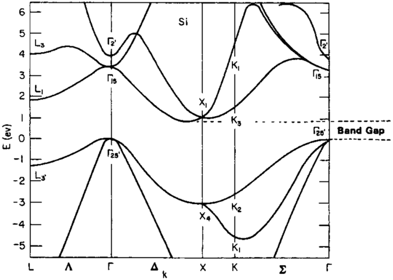
$$\psi_{\boldsymbol{k}}(\boldsymbol{n},\beta) = \psi_\beta(\boldsymbol{k})\mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{x_n}}, \qquad \sum_{\boldsymbol{n},\beta} H_{\boldsymbol{m}\alpha;\boldsymbol{n}\beta}\ \psi_{\boldsymbol{k}}(\boldsymbol{n},\beta) = \epsilon_{\boldsymbol{k}}\psi_k(\boldsymbol{m},\alpha)$$

- The energy bands $\epsilon_{\boldsymbol{k}}$ are eigenvalues of $M_{\alpha\beta}(\boldsymbol{k})$

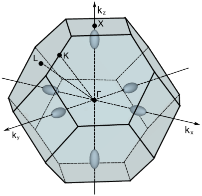
$$\sum_\beta M_{\alpha\beta}(\boldsymbol{k})\psi_\beta(\boldsymbol{k}) = \epsilon_k\psi_\alpha(\boldsymbol{k}),$$

$$M_{\alpha\beta}(\boldsymbol{k}) = -\sum_{\Delta\boldsymbol{n}} t^{\Delta\boldsymbol{n}}_{\alpha\beta}\,\mathrm{e}^{-\mathrm{i}\,\boldsymbol{x}_{\Delta\boldsymbol{n}}\cdot\boldsymbol{k}}$$

Si bands



- Number of bands = number of orbitals in a unit cell.

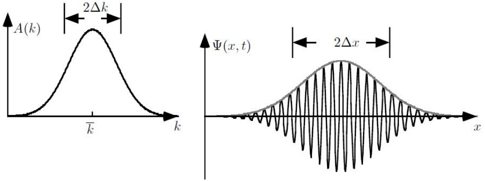


Dynamics of an electron in semiconductor

The standard theory

- Quantum dynamics: $H(\hat{\boldsymbol{p}}) = \epsilon(\hat{\boldsymbol{p}})$, $\hat{p} = -\mathrm{i}\hbar\boldsymbol{\partial} \to$
  A plane wave $\mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{x}}\psi_\alpha(\boldsymbol{k}) = \mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{x}}|\psi(\boldsymbol{k})\rangle$
  evolves as $\mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{x}}\mathrm{e}^{-\mathrm{i}\,\frac{\epsilon(\hbar\boldsymbol{k})}{\hbar}t}|\psi(\boldsymbol{k})\rangle$.
  With potential term, the Hamiltonian is changed to
  $H(\hat{\boldsymbol{p}},\hat{\boldsymbol{x}}) = \epsilon(\hat{\boldsymbol{p}}) + V(\hat{\boldsymbol{x}})$, where $[\hat{p}^i,\hat{x}^j] = -\mathrm{i}\hbar\delta_{ij}$.
- Classical dynamics: $\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{O}\rangle = \frac{\mathrm{i}}{\hbar}\langle[H,\hat{O}]\rangle \to$

$$\dot{\boldsymbol{p}} = -\frac{\partial H(\boldsymbol{p},\boldsymbol{x})}{\partial\boldsymbol{x}}, \qquad \dot{\boldsymbol{x}} = \frac{\partial H(\boldsymbol{p},\boldsymbol{x})}{\partial\boldsymbol{p}}.$$

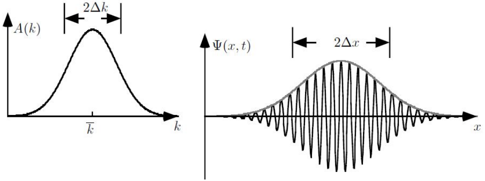


Dynamics of an electron in semiconductor

The standard theory

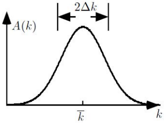
- Quantum dynamics: $H(\hat{\boldsymbol{p}}) = \epsilon(\hat{\boldsymbol{p}})$, $\hat{p} = -\mathrm{i}\hbar\boldsymbol{\partial} \to$
  A plane wave $\mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{x}}\psi_\alpha(\boldsymbol{k}) = \mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{x}}|\psi(\boldsymbol{k})\rangle$
  evolves as $\mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{x}}\mathrm{e}^{-\mathrm{i}\,\frac{\epsilon(\hbar\boldsymbol{k})}{\hbar}t}|\psi(\boldsymbol{k})\rangle$.
  With potential term, the Hamiltonian is changed to
  $H(\hat{\boldsymbol{p}}, \hat{\boldsymbol{x}}) = \epsilon(\hat{\boldsymbol{p}}) + V(\hat{\boldsymbol{x}})$, where $[\hat{p}^i, \hat{x}^j] = -\mathrm{i}\hbar\delta_{ij}$.
- Classical dynamics: $\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{O}\rangle = \frac{\mathrm{i}}{\hbar}\langle[H, \hat{O}]\rangle \to$

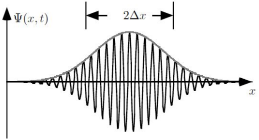
$$\dot{\boldsymbol{p}} = -\frac{\partial H(\boldsymbol{p}, \boldsymbol{x})}{\partial \boldsymbol{x}}, \qquad \dot{\boldsymbol{x}} = \frac{\partial H(\boldsymbol{p}, \boldsymbol{x})}{\partial \boldsymbol{p}}.$$



- *The standard theory is wrong.* $V(\hat{\boldsymbol{x}})$ *is wrong*

Obtain classical EOM of an electron in a band





- Consider wavepacket with space-time dependent spin

$$|\psi_{\boldsymbol{x}_0,\boldsymbol{k}_0}\rangle = \left(\frac{\alpha}{\pi}\right)^{1/4} \mathrm{e}^{\mathrm{i}\,\boldsymbol{k}_0\boldsymbol{x}}\,\mathrm{e}^{-\frac{1}{2}\alpha(\boldsymbol{x}-\boldsymbol{x}_0)^2}|\psi(\boldsymbol{k}_0)\rangle$$

Phase space Lagrangian

$$\mathcal{L} = \langle\psi_{\boldsymbol{x}_0(t),\boldsymbol{k}_0(t)}|\,\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t} - H|\psi_{\boldsymbol{x}_0(t),\boldsymbol{k}_0(t)}\rangle$$

$$= \hbar\underbrace{\boldsymbol{a}'}_{=0}\cdot\dot{\boldsymbol{x}}_0 + \hbar\underbrace{\boldsymbol{a}''}_{-\boldsymbol{x}_0}\cdot\dot{\boldsymbol{k}}_0 + \hbar\underbrace{\tilde{\boldsymbol{a}}(\boldsymbol{k}_0)}_{-\mathrm{i}\,\langle\psi|\partial_{\boldsymbol{k}_0}|\psi\rangle}\cdot\dot{\boldsymbol{k}}_0 - \frac{\hbar^2\boldsymbol{k}_0^2}{2m_n} - |\mu_n\boldsymbol{B}(\boldsymbol{x}_0)|$$

$$= -\hbar\boldsymbol{x}_0\cdot\dot{\boldsymbol{k}}_0 + \hbar\tilde{\boldsymbol{a}}(\boldsymbol{k}_0)\cdot\dot{\boldsymbol{k}}_0 - \frac{\hbar^2\boldsymbol{k}_0^2}{2m_n} + |\mu_n\boldsymbol{B}(\boldsymbol{x}_0)|$$

$$\approx \boldsymbol{p}_0\cdot\dot{\boldsymbol{x}}_0 + \tilde{\boldsymbol{a}}(\boldsymbol{p}_0/\hbar)\cdot\dot{\boldsymbol{p}}_0 - \frac{\boldsymbol{p}_0^2}{2m_n} - V(\boldsymbol{x}_0)$$

Obtain classical EOM of an electron in a band

- The $\boldsymbol{k}$-space connection (vector potential) in Brillouin zone.

$$\mathrm{i}\,\tilde{\boldsymbol{a}}(\boldsymbol{k}) = \langle \psi(\boldsymbol{k})|\partial_{\boldsymbol{k}}|\psi(\boldsymbol{k})\rangle$$

- For $S = \int \mathrm{d}t\ [\boldsymbol{p}\cdot\dot{\boldsymbol{x}} + \tilde{\boldsymbol{a}}(\boldsymbol{p}/\hbar)\cdot\dot{\boldsymbol{p}} - \frac{\boldsymbol{p}^2}{2m_n} - V(\boldsymbol{x})]$

  From $\int \mathrm{d}t\ \delta(\tilde{a}_i(\boldsymbol{p}/\hbar)\dot{p}^i) = \int \mathrm{d}t\ [\delta p^j(\partial_{p_j}\tilde{a}_i)\dot{p}^i - \dot{\tilde{a}}_i(\boldsymbol{p}/\hbar)\delta p^i]$

  $\delta S = \int \mathrm{d}t\ \delta p_i[\dot{x}^i - \frac{p_i}{m_n} + \hbar^{-1}(\partial_{k_i}\tilde{a}_j)\dot{p}^j - \hbar^{-1}(\partial_{k_j}\tilde{a}_i)\dot{p}^j] + \delta x^i[-\dot{p}_i - \partial_i V]$

  we obtain the phase space equation of motion

$$\dot{x}^i = \frac{p_i}{m_n} - \underbrace{\hbar^{-1}(\partial_{k_i}\tilde{a}_j - \partial_{k_j}\tilde{a}_i)\dot{p}^j}_{\text{Velocity correction}} = \frac{p_i}{m_n} - \hbar^{-1}\tilde{b}_{IJ}\dot{p}^j, \qquad \dot{p}_i = -\partial_i V$$

  where $\tilde{b}_{IJ} = \partial_{k_i}\tilde{a}_j - \partial_{k_j}\tilde{a}_i$ is the $\boldsymbol{k}$-space "magnetic" field (geometric curvature).

Qian Niu

The $\boldsymbol{k}$-space connection (*ie* the $\boldsymbol{k}$-space magnetic field) also modifies the equation of motion

The correct classical EOM of an electron in a band

$$L = \boldsymbol{p}\cdot\dot{\boldsymbol{x}} + \frac{e}{c}\boldsymbol{A}(\boldsymbol{x})\cdot\dot{\boldsymbol{x}} + \tilde{\boldsymbol{a}}(\boldsymbol{p}/\hbar)\cdot\dot{\boldsymbol{p}} - \frac{\boldsymbol{p}^2}{2m_n} - V(\boldsymbol{x})$$

$$= \hbar[\boldsymbol{k}\cdot\dot{\boldsymbol{x}} + \boldsymbol{a}(\boldsymbol{x})\cdot\dot{\boldsymbol{x}} + \tilde{\boldsymbol{a}}(\boldsymbol{k})\cdot\dot{\boldsymbol{k}}] - \frac{\boldsymbol{p}^2}{2m_n} - V(\boldsymbol{x})$$

The real equation of motion in semiconductor

$$\dot{p}_i = -\frac{\partial V}{\partial x^i} + \frac{e}{c}B_{ij}\dot{x}^j = F_i, \quad \dot{x}_i = \frac{\partial \epsilon}{\partial p_i} - \hbar^{-1}\tilde{b}_{ij}(\boldsymbol{k})\dot{p}_j.$$

F_i include both potential force and Lorentz force.

- Phase space curvature ($I = x^1, x^2, x^3, k^1, k^2, k^3$)

$$(b_{IJ}) = \begin{pmatrix} b_{ij} & \delta_{ij} \\ -\delta_{ij} & \tilde{b}_{ij} \end{pmatrix}, \quad \begin{pmatrix} 0 & -\delta_{ij} \\ \delta_{ij} & 0 \end{pmatrix}\begin{pmatrix} b_{ij} & \delta_{ij} \\ -\delta_{ij} & \tilde{b}_{ij} \end{pmatrix} = \begin{pmatrix} \delta_{ij} & \tilde{b}_{ij} \\ b_{ij} & \delta_{ij} \end{pmatrix}$$

$$\log \mathrm{Det}\begin{pmatrix} \delta_{ij} & \tilde{b}_{ij} \\ b_{ij} & \delta_{ij} \end{pmatrix} = \mathrm{Tr}\log\begin{pmatrix} \delta_{ij} & \tilde{b}_{ij} \\ b_{ij} & \delta_{ij} \end{pmatrix} = 2b_{ij}\tilde{b}_{ji} + O(b_{ik}\tilde{b}_{kj})^2$$

$$\mathrm{Pf}\begin{pmatrix} b_{ij} & \delta_{ij} \\ -\delta_{ij} & \tilde{b}_{ij} \end{pmatrix} \equiv \mathrm{Pf}(b, \tilde{b}) = 1 + b_{ij}\tilde{b}_{ji} + O(b_{ik}\tilde{b}_{kj})^2.$$

Compare with Newton's law

From the EOM

$$\dot{k}_i = \hbar^{-1} F_i, \qquad \dot{x}_i = \hbar^{-1}\frac{\partial \epsilon}{\partial k_i} - \tilde{b}_{ij}(\boldsymbol{k})\dot{k}_j = \hbar^{-1}\frac{\partial \epsilon}{\partial k_i} - \hbar^{-1}\tilde{b}_{ij}(\boldsymbol{k})F_j$$

and assume $H = \frac{\hbar^2 \boldsymbol{k}^2}{2m} + V(\boldsymbol{x})$, $\tilde{b}_{ij} = \tilde{b}_{ij}(\boldsymbol{k})$, we obtain

$$\begin{aligned} \ddot{x}^i &= \hbar^{-2}(\partial_{k_i}\partial_{k_j} H)F_j - \hbar^{-1}\tilde{b}_{ij}\dot{F}_j - \hbar^{-2}\partial_{k_l}\tilde{b}_{ij}F_jF_l \\ \text{or} \quad \ddot{x}^i &= (\partial_{p_i}\partial_{p_j} H)F_j - D_{ij}\dot{F}_j - \partial_{k_l}D_{ij}F_jF_l \\ &= m^{-1}F_i - D_{ij}\dot{F}_j - \partial_{k_l}D_{ij}F_jF_l \end{aligned}$$

where $p_i = \hbar k_i,\ D_{ij} = \hbar^{-1}\tilde{b}_{ij}$.
We obtain correction to the Newton law $-D_{ij}\dot{F}_j - \partial_{p_l}D_{ij}F_jF_l$.

$\frac{\boldsymbol{p}^2}{2m} \to \sqrt{m^2c^4 + c^2\boldsymbol{p}^2}$ *is the relativistic correction.*

AC conductivity (from classical Drude model)

First way to include a friction force

$$F_i \to F_i - \gamma \dot{x}^i$$

We obtain

$$\ddot{x}^i = m^{-1}(F_i - \gamma \dot{x}^i) - D_{ij}(\dot{F}_j - \gamma \ddot{x}^i) - \partial_{P_l} D_{ij}(F_j - \gamma \dot{x}^j)(F_l - \gamma \dot{x}^l)$$

- Assume $\partial_{P_l} D_{ij} = 0$ and go to ω-space $\boldsymbol{x} = \boldsymbol{x}_\omega \mathrm{e}^{-\mathrm{i}\omega t}$:

$$[-\omega^2(\delta_{ij} - \gamma D_{ij}) - \mathrm{i}\omega\gamma m^{-1}\delta_{ij}]x^j_\omega = [m^{-1}\delta_{ij} + \mathrm{i}\, D_{ij}]F_j$$
$$\boldsymbol{x}_\omega = [-\omega^2(m - \gamma m D) - \mathrm{i}\omega\gamma]^{-1}(1 + \mathrm{i}\omega m D)\boldsymbol{F}_\omega$$
$$\boldsymbol{v}_\omega = [\gamma - \mathrm{i}\omega m(1 - \gamma D)]^{-1}(1 + \mathrm{i}\omega m D)\boldsymbol{F}_\omega$$

Effect of D_{ij} disappear for DC conductance.

AC conductivity (from classical Drude model)

Second way to include a friction force

$$F_i \to F_i - \gamma \partial_{p_i} H = F_i - \gamma m^{-1} p_i$$

Still assume $\partial_{p_l} D_{ij} = 0$:

$$\dot{\boldsymbol{x}} = \partial_{\boldsymbol{p}} H - D(\boldsymbol{F} - \gamma m^{-1}\boldsymbol{p}) = (1+\gamma D) m^{-1}\boldsymbol{p} - D\boldsymbol{F}$$
$$\dot{\boldsymbol{p}} = \boldsymbol{F} - \gamma m^{-1}\boldsymbol{p}.$$

- Go to ω-space $\boldsymbol{x} = \boldsymbol{x}_\omega \mathrm{e}^{-\mathrm{i}\omega t}$: $\quad -\mathrm{i}\omega \boldsymbol{p}_\omega = \boldsymbol{F}_\omega - \gamma m^{-1}\boldsymbol{p}_\omega$

$$\begin{aligned}
\boldsymbol{v}_\omega = -\mathrm{i}\omega \boldsymbol{x}_\omega &= (1+\gamma D) m^{-1}\boldsymbol{p}_\omega - D\boldsymbol{F}_\omega \\
&= (1+\gamma D) m^{-1} \frac{1}{\gamma m^{-1} - \mathrm{i}\omega} \boldsymbol{F}_\omega - D\boldsymbol{F}_\omega \\
&= (1+\gamma D) \frac{1}{\gamma - \mathrm{i}\omega m} \boldsymbol{F}_\omega - D\boldsymbol{F}_\omega \\
&= (1+\mathrm{i}\omega D m)(\gamma - \mathrm{i}\omega m)^{-1} \boldsymbol{F}_\omega
\end{aligned}$$

Effect of D_{ij} still disappear for DC conductance, the result is different from the first one.

Transport: Boltzmann equation (fluid equ. in phase space)

In fact, D_{ij} has effect on DC conductance,
at least for **quantum Fermi gas.**

- Phase space is parametrized by $\xi^I = x^1, x^2, x^3, k^1, k^2, k^3$

$$L(\dot{\xi}^I, \xi^I) = \hbar a_I \dot{\xi}^I - H, \qquad \hbar b_{IJ}\dot{\xi}^J = \frac{\partial H}{\partial \xi^I}, \qquad b_{IJ} = \partial_I a_J - \partial_J a_I$$

- We introduce phase space density distribution

$$\mathrm{d}N = g(\xi^I)\mathrm{Pf}[b(\xi^I)]\frac{\mathrm{d}^n\xi^I}{(2\pi)^{n/2}}$$

g is the number per orbital.

- Local equilibrium distribution

$$g_0(\xi^I) = \frac{1}{\mathrm{e}^{\beta(\xi^I)[H(\xi^I)-\mu]}+1}, \qquad \text{for fermions}$$

$$g_0(\xi^I) = \frac{1}{\mathrm{e}^{\beta(\xi^I)[H(\xi^I)-\mu]}-1}, \qquad \text{for bosons}$$

$$g_0(\xi^I) = \mathrm{e}^{-\beta(\xi^I)[H(\xi^I)-\mu]}, \qquad \text{for classical particles}$$

Hydrodynamic equation of motion

- Consider a small cluster of gas, that evolve from time t to $\tilde{t}$

$$\mathrm{d}N = \mathrm{d}\tilde{N} \quad \text{or} \quad g(\xi^I)\mathrm{Pf}[b(\xi^I)]\frac{\mathrm{d}^n\xi^I}{(2\pi)^{n/2}} = g(\tilde{\xi}^I)\mathrm{Pf}[b(\tilde{\xi}^I)]\frac{\mathrm{d}^n\tilde{\xi}^I}{(2\pi)^{n/2}}$$

Due to Liouville's theorm $\mathrm{Pf}[b(\xi^I)]\mathrm{d}^n\xi^I = \mathrm{Pf}[b(\tilde{\xi}^I)]\mathrm{d}^n\tilde{\xi}^I$, we have

$$g(\xi^I) = g(\tilde{\xi}^I) \quad \text{or} \quad \frac{\mathrm{d}}{\mathrm{d}t}g[\xi^I(t)] = 0$$

We obtain **hydrodynamic equation**

$$\frac{\mathrm{d}}{\mathrm{d}t}g[\xi^I(t)] = 0 \quad \to \quad \frac{\partial g}{\partial t} + \dot{\xi}^I\partial_I g = \frac{\partial g}{\partial t} + \hbar b^{IJ}\partial_J H \partial_I g = 0$$

- Consistent with the conservation of particle number ($b_{IJ} = const.$):

$$\frac{\partial g}{\partial t} + \partial_I \mathcal{J}^I = 0, \quad \text{current: } \mathcal{J}^I = g\dot{\xi}^I = \hbar g\ b^{IJ}\partial_J H$$

$$0 = \frac{\partial g}{\partial t} + \partial_I \mathcal{J}^I = \frac{\partial g}{\partial t} + \hbar b^{IJ}\partial_I g \partial_J H + \hbar b^{IJ} g \partial_I \partial_J H$$

$$= \frac{\partial g}{\partial t} + \hbar b^{IJ}\partial_I g \partial_J H$$

The conservation of particle number for $b_{IJ} \neq const.$

Assume for phase space coordinates $\tilde{\xi}^I$, $\tilde{b}_{IJ} = const.$

- Hydrodynamic EOM and conservation equation:

$$\frac{\partial \tilde{g}}{\partial t} + \dot{\tilde{\xi}}^I \tilde{\partial}_I \tilde{g} = \frac{\partial \tilde{g}}{\partial t} + \hbar \tilde{b}^{IJ} \tilde{\partial}_J H \tilde{\partial}_I \tilde{g} = 0$$

$$\frac{\partial \tilde{g}}{\partial t} + \tilde{\partial}_I \tilde{\mathcal{J}}^I = 0, \quad \tilde{\mathcal{J}}^I = \tilde{g} \dot{\tilde{\xi}}^I, \qquad \dot{\tilde{\xi}}^I = \hbar \tilde{b}^{IJ} \tilde{\partial}_J H$$

- **Change of coordinates**: $\xi^I = \xi^I(\tilde{\xi}^I)$

$$g(\xi^I) = \tilde{g}(\tilde{\xi}^I), \quad \partial_I = \frac{\partial \tilde{\xi}^J}{\partial \xi^I} \tilde{\partial}_J, \quad \dot{\xi}^I = \frac{\partial \xi^I}{\partial \tilde{\xi}^J} \dot{\tilde{\xi}}^J, \quad \mathcal{J}^I = \frac{\partial \xi^I}{\partial \tilde{\xi}^J} \tilde{\mathcal{J}}^J,$$

$$b_{IJ} = \frac{\partial \tilde{\xi}^K}{\partial \xi^I} \frac{\partial \tilde{\xi}^L}{\partial \xi^J} \tilde{b}_{KL}, \qquad b^{IJ} = \frac{\partial \xi^I}{\partial \tilde{\xi}^K} \frac{\partial \xi^J}{\partial \tilde{\xi}^L} \tilde{b}^{KL}$$

\- The subscript and superscript indecate how the quantity transforms under the coordinate transformation.

- The form of the hydrodynamic EOM remain unchanged:

$$\frac{\partial g}{\partial t} + \dot{\xi}^I \partial_I g = \frac{\partial g}{\partial t} + \hbar b^{IJ} \partial_J H \partial_I g = 0$$

The conservation of particle number for $b_{IJ} \neq const.$

- The form of the conservation equation is changed:

$$0 = \frac{\partial g}{\partial t} + \frac{\partial \xi^K}{\partial \tilde{\xi}^I}\Big(\partial_K \frac{\partial \tilde{\xi}^I}{\partial \xi^L}\mathcal{J}^L\Big) = \frac{\partial g}{\partial t} + \partial_I \mathcal{J}^I + \frac{\partial \xi^K}{\partial \tilde{\xi}^I}\Big(\partial_K \frac{\partial \tilde{\xi}^I}{\partial \xi^L}\Big)\mathcal{J}^L$$

$$= \frac{\partial g}{\partial t} + \partial_I \mathcal{J}^I + \frac{\partial \xi^K}{\partial \tilde{\xi}^I}\Big(\partial_L \frac{\partial \tilde{\xi}^I}{\partial \xi^K}\Big)\mathcal{J}^L$$

In fact: $\frac{\partial \xi^K}{\partial \tilde{\xi}^I}\Big(\partial_L \frac{\partial \tilde{\xi}^I}{\partial \xi^K}\Big) = \mathrm{Det}^{1/2}(b^{IJ})\partial_K \mathrm{Det}^{1/2}(b_{IJ})$, since the RHS

$= \mathrm{Det}(\frac{\partial \xi^J}{\partial \tilde{\xi}^I})\mathrm{Det}^{1/2}(\tilde{b}^{IJ})\partial_K\Big[\mathrm{Det}(\frac{\partial \tilde{\xi}^I}{\partial \xi^J})\mathrm{Det}^{1/2}(\tilde{b}_{IJ})\Big] = \mathrm{Det}(\frac{\partial \xi^J}{\partial \tilde{\xi}^I})\partial_K \mathrm{Det}(\frac{\partial \tilde{\xi}^I}{\partial \xi^J})$

We also have (let $M_{IJ} = \frac{\partial \tilde{\xi}^I}{\partial \xi^J}$)

$\mathrm{Det}(M^{IJ})\delta\mathrm{Det}(M_{IJ}) = \mathrm{Det}(M^{IJ})\mathrm{Det}(M_{IJ} + \delta M_{IJ}) - 1$

$= \mathrm{Det}(\delta_{IJ} + M^{IK}\delta M_{KJ}) - 1 = M^{IK}\delta M_{KI}$

Conservation equation: (not just $\frac{\partial g}{\partial t} + \partial_I \mathcal{J}^I = 0$)

$$\frac{\partial g}{\partial t} + \partial_I \mathcal{J}^I + \frac{1}{\mathrm{Pf}(\hat{b})}\big[\partial_I \mathrm{Pf}(\hat{b})\big]\mathcal{J}^I = \frac{\partial g}{\partial t} + \frac{1}{\mathrm{Pf}(\hat{b})}\partial_I\big[\mathrm{Pf}(\hat{b})\mathcal{J}^I\big] = 0$$

Conservation equation = Hydrodynamic equation

$$0 = \frac{\partial g}{\partial t} + \frac{1}{\mathrm{Pf}(\hat{b})}\partial_I\left[\mathrm{Pf}(\hat{b})\mathcal{J}^I\right] = \frac{\partial g}{\partial t} + \frac{1}{\mathrm{Pf}(\hat{b})}\partial_I\left[\mathrm{Pf}(\hat{b})\ g\ \hbar b^{IJ}\partial_J H\right]$$

$$= \frac{\partial g}{\partial t} + \hbar b^{IJ}\partial_I g \partial_J H + \hbar g \partial_J H \underbrace{\frac{1}{\mathrm{Pf}(\hat{b})}\partial_I\left[\mathrm{Pf}(\hat{b}) b^{IJ}\right]}_{=0}$$

We first note that $0 = \partial_M(b^{IK}b_{KL}) = (\partial_M b^{IK})b_{KL} + b^{IK}(\partial_M b_{KL})$
$\to 0 = \partial_M b^{IJ} + b^{IK}(\partial_M b_{KL})b^{LJ}$
This allows us to obtain

$$\frac{\partial_I\left[\mathrm{Pf}(\hat{b})b^{IJ}\right]}{\mathrm{Pf}(\hat{b})} = \frac{b^{KL}\partial_I b_{LK}}{2}b^{IJ} + \partial_I b^{IJ} = \frac{b^{KL}b^{IJ}\partial_I b_{LK}}{2} - b^{IK}(\partial_I b_{KL})b^{LJ}$$

$$= \frac{b^{KL}b^{IJ}\partial_I(\partial_L a_K - \partial_K a_L)}{2} - b^{IK}b^{LJ}\partial_I(\partial_K a_L - \partial_L a_K)$$

$$= b^{KL}b^{IJ}\partial_I\partial_L a_K + b^{IK}b^{LJ}\partial_I\partial_L a_K = b^{KL}b^{IJ}\partial_I\partial_L a_K + b^{LK}b^{IJ}\partial_L\partial_I a_K = 0$$

We recover the hydrodynamic equation $\frac{\partial g}{\partial t} + \hbar b^{IJ}\partial_I g \partial_J H = 0$.

Adding dissipation – difffusion in phase space

The enviromental influence only change ξ^I slightly each time.

Diffusion current

$$\mathcal{J}^I_{\text{diff}} = \gamma^{IJ}\frac{\partial g}{\partial \xi^J} = -\gamma^{IJ}\partial_J g. \qquad \text{(Should } \gamma^{IJ} \text{ be symmetric?)}$$

New EOM (new continuity equation)

$$\frac{\partial g}{\partial t} + \frac{1}{\text{Pf}(\hat{b})}\partial_I\left[\text{Pf}(\hat{b})\ g\dot{\xi}^I\right] - \frac{1}{\text{Pf}(\hat{b})}\partial_I\left[\text{Pf}(\hat{b})\mathcal{J}^I_{\text{diff}}\right] = 0$$

$$\text{or} \qquad \frac{\partial g}{\partial t} + \dot{\xi}^I\partial_I g = \frac{1}{\text{Pf}(\hat{b})}\partial_I\left[\text{Pf}(\hat{b})\gamma^{IJ}\partial_J g\right]$$

- But the above difusion model does not satisfy detail balance. It assume the transition rates caused by environmntal influence between two states A, B to be the same in either direction: $t_{A\to B} = t_{B\to A}$. Such a transition rates give rise to equilibrium probability distribution that satisfies $P_A = P_B$ regardless the energy difference $E_A - E_B$ of the two states. This coresponds to $T = \infty$ case. Indeed the above diffusion model tends to make g to be uniform in phase space, which is the $T = \infty$ case.

Adding dissipation – difffusion in phase space

How to find a difussion model that satisfy detail balance?

How to find a difussion model that make g to evolve into the equilibrium distributions for a finite temperature T:

$$g_0(\xi^I) = \frac{1}{e^{\beta[H(\xi^I)-\mu]} + 1}, \qquad \text{for fermions}$$

$$g_0(\xi^I) = \frac{1}{e^{\beta[H(\xi^I)-\mu]} - 1}, \qquad \text{for bosons}$$

$$g_0(\xi^I) = e^{-\beta[H(\xi^I)-\mu]}, \qquad \text{for classical particles}$$

Diffusion current

$$\mathcal{J}^I_{\text{diff}} = -\gamma^{IJ} g \partial_J (\log g + \beta H), \qquad \text{for classical particles}$$

$$\mathcal{J}^I_{\text{diff}} = -\gamma^{IJ} g(1-g) \partial_J [-\log(g^{-1}-1) + \beta H], \qquad \text{for fermions}$$

$$\mathcal{J}^I_{\text{diff}} = -\gamma^{IJ} g(1+g) \partial_J [-\log(g^{-1}+1) + \beta H], \qquad \text{for bosons}$$

Hydrodynamics in phase space with dissipation

For classical particles (high temperature limit)

$$\frac{\partial g}{\partial t} + \dot{\xi}^I \partial_I g = \frac{1}{\mathrm{Pf}(\hat{b})} \partial_I \left[\mathrm{Pf}(\hat{b}) \gamma^{IJ} g \partial_J (\log g + \beta H) \right]$$

For fermions

$$\frac{\partial g}{\partial t} + \dot{\xi}^I \partial_I g = \frac{1}{\mathrm{Pf}(\hat{b})} \partial_I \left[\mathrm{Pf}(\hat{b}) \gamma^{IJ} g(1-g) \partial_J (\log \frac{g}{1-g} + \beta H) \right]$$

For bosons

$$\frac{\partial g}{\partial t} + \dot{\xi}^I \partial_I g = \frac{1}{\mathrm{Pf}(\hat{b})} \partial_I \left[\mathrm{Pf}(\hat{b}) \gamma^{IJ} g(1+g) \partial_J (\log \frac{g}{1+g} + \beta H) \right]$$

- The equilibrium distribution g_0 satisfies the above EOM.
- The above diffusion term only incorporates the particle number conservation, not energy conservation, since we consider an open system and assume T to be fixed.
  How to include energy conservation for a closed system?

Go to $\xi^I = \boldsymbol{x}, \boldsymbol{k}$ phase space

But the scattering by impurities and other particles usually cause large $\Delta \boldsymbol{k}$. Diffusion only happen in $\boldsymbol{x}$ space. In $\boldsymbol{k}$-space, we have have something more dramatic.

$$L = \hbar[\boldsymbol{k} \cdot \dot{\boldsymbol{x}} + \boldsymbol{a}(\boldsymbol{x}) \cdot \dot{\boldsymbol{x}} + \tilde{\boldsymbol{a}}(\boldsymbol{k}) \cdot \dot{\boldsymbol{k}}] - E(\boldsymbol{k}, \boldsymbol{x}), \quad E(\boldsymbol{k}, \boldsymbol{x}) = \epsilon(\boldsymbol{k}) + V(\boldsymbol{x})$$

$$\hbar \dot{k}_i = -\frac{\partial E}{\partial x^i} + \underbrace{\hbar b_{ij}}_{=\frac{e}{c} B_{ij}} \dot{x}^j, \qquad \hbar \dot{x}_i = \frac{\partial E}{\partial k_i} - \hbar \tilde{b}_{ij}(\boldsymbol{k}) \dot{k}_j.$$

- $(\boldsymbol{x}, \boldsymbol{k})$-density distribution function

$$g(\boldsymbol{x}, \boldsymbol{k}, t) : \mathrm{d}N = g(\boldsymbol{x}, \boldsymbol{k}, t) \ \mathrm{Pf}(b, \tilde{b}) \frac{\mathrm{d}^3 \boldsymbol{x} \, \mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3}$$

g is the number per orbital, and $\mathrm{Pf}(b, \tilde{b}) = 1 + b_{ij} \tilde{b}_{ji} + \cdots$.

- Local equilibrium distribution

$$g_0(\boldsymbol{x}, \boldsymbol{k}) = \frac{1}{\mathrm{e}^{\beta(\boldsymbol{x})[E(\boldsymbol{k}, \boldsymbol{x}) - \mu(\boldsymbol{x})]} + 1}, \qquad \text{for fermions}$$

$$g_0(\boldsymbol{x}, \boldsymbol{k}) = \frac{1}{\mathrm{e}^{\beta(\boldsymbol{x})[E(\boldsymbol{k}, \boldsymbol{x}) - \mu(\boldsymbol{x})]} - 1}, \qquad \text{for bosons}$$

$$g_0(\boldsymbol{x}, \boldsymbol{k}) = \mathrm{e}^{-\beta(\boldsymbol{x})[E(\boldsymbol{k}, \boldsymbol{x}) - \mu(\boldsymbol{x})]}, \qquad \text{for classical particles}$$

Adding dissipation – relaxationtime approximation

- We will model large Δk redistribution in $\boldsymbol{k}$-space by

$$\frac{\partial g}{\partial t} + \dot{\xi}^I \partial_I g = \frac{\partial g}{\partial t} + \dot{\boldsymbol{x}} \cdot \frac{\partial g}{\partial \boldsymbol{x}} + \dot{\boldsymbol{k}} \cdot \frac{\partial g}{\partial \boldsymbol{k}} = -\frac{1}{\tau}(g - g_0)$$

\- $\frac{\mathrm{d}g}{\mathrm{d}t} = \frac{1}{\tau}(g - g_0)$ corresponds to the change of g caused by scattering process in $\boldsymbol{k}$ space. It should conserve the $\boldsymbol{x}$-space particle density $n(\boldsymbol{x}) = \int \mathrm{Pf}(b, \tilde{b}) \frac{\mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3}\ g$. Thus the chemical potential $\mu(\boldsymbol{x})$ in g_0 is chosen to make g_0 to satisfy

$$\delta n(\boldsymbol{x}) = \int \mathrm{Pf}(b, \tilde{b}) \mathrm{d}^3 \boldsymbol{k}\ (g - g_0) = 0.$$

\- No particle diffusion in $\boldsymbol{x}$-space.

- To conserve the energy density in $\boldsymbol{x}$-space $n_E(\boldsymbol{x}) = \int \mathrm{Pf}(b, \tilde{b}) \frac{\mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3}\ E(\boldsymbol{x}, \boldsymbol{k}) g$, we choose temperature $T(\boldsymbol{x})$ such that

$$\delta n_E(\boldsymbol{x}) = \int \mathrm{Pf}(b, \tilde{b}) \mathrm{d}^3 \boldsymbol{k}\ E(\boldsymbol{x}, \boldsymbol{k})(g - g_0) = 0.$$

Linear responce in steady state

- Steady state: $\frac{\partial g}{\partial t} = 0$ or $\quad \dot{\boldsymbol{x}} \cdot \frac{\partial g}{\partial \boldsymbol{x}} + \dot{\boldsymbol{k}} \cdot \frac{\partial g}{\partial \boldsymbol{k}} = -\frac{1}{\tau}(g - g_0)$
  with EOM for particles $\hbar \dot{k}_i = -\frac{\partial V}{\partial x^i} + \hbar b_{ij} \dot{x}^j, \ \hbar \dot{x}_i = \frac{\partial \epsilon}{\partial k_i} - \hbar \tilde{b}_{ij}(\boldsymbol{k}) \dot{k}_j$
  and $g_0(\boldsymbol{x}, \boldsymbol{k}) = 1/(\mathrm{e}^{\beta(\boldsymbol{x})[\epsilon(\boldsymbol{k}) + V(\boldsymbol{x}) - \mu(\boldsymbol{x})]} + 1)$
- When $\partial_{\boldsymbol{x}} V = 0, \ b_{ij} = 0, \ \ \partial_{\boldsymbol{x}} \mu = 0, \ \partial_{\boldsymbol{x}} \beta(\boldsymbol{x}) = 0$,
  g_0 satisfies the EOM, since $\dot{\boldsymbol{k}} = 0$, $\frac{\partial g_0}{\partial \boldsymbol{x}} = \frac{\partial g_0}{\partial t} = 0$
- Linear responce: first order in

$$\dot{\boldsymbol{k}} \sim \partial_{\boldsymbol{x}} V, b_{ij}, \qquad \partial_{\boldsymbol{x}} g_0 \sim \partial_{\boldsymbol{x}} \underbrace{(V - \mu)}_{-\bar{\mu}}, \partial_{\boldsymbol{x}} \beta \qquad \delta g = g - g_0.$$

- **Linear response for steady state**

$$\delta g + \tau \hbar^{-1} \partial_{k_i} \epsilon \partial_{x_i} \delta g = -\tau [\hbar^{-1} \partial_{k_i} \epsilon \partial_{x_i} g_0 + \dot{k}_i \partial_{k_i} g_0]$$

$$\text{or} \quad \delta g + \tau v^i \partial_{x_i} \delta g = -\tau [v^i \partial_{x_i} g_0 + \dot{k}_i \partial_{k_i} g_0], \qquad v^i = \hbar^{-1} \partial_{k_i} \epsilon.$$

Assume $\tau v^i \partial_{x_i} \delta g \ll \delta g$ and since $\hbar \dot{k}_i = e E_i + \hbar b_{ij} v^j$:

$$\delta g = -\tau v^i \partial_{x_i} g_0 + \frac{\tau}{\hbar}(e E_i + \hbar b_{ij} v^j) \partial_{k_i} g_0, \qquad g_0 = \frac{1}{\mathrm{e}^{\beta(\boldsymbol{x})[\epsilon(\boldsymbol{k}) - \bar{\mu}(\boldsymbol{x})]} + 1}$$

2D conductivity from $\boldsymbol{k}$-space "magnetic" field $\tilde{b}_{ij}$

Assume real space magnetic field $b_{ij} = 0$ and $T(\boldsymbol{x})$, $\bar{\mu}(\boldsymbol{x})$ are independent of $\boldsymbol{x}$:

$$\delta g = \tau e E_i \frac{\partial \epsilon}{\hbar \partial k_i} \frac{\partial g_0}{\partial \epsilon} = \tau e E_i v^i \frac{\partial g_0}{\partial \epsilon}$$

The current ($\mathrm{Pf}(b_{ij}, \tilde{b}_{ij}) = \mathrm{Pf}(0, \tilde{b}_{ij}) = 1$)

$$J^i = \int \frac{\mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3} e \dot{x}^i g = \int \frac{\mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3} (e v^i - e \tilde{b}_{ij}\ \hbar^{-1} e E_j)(g_0 + \tau e E_i v^i \frac{\partial g_0}{\partial \epsilon})$$

Note that

$$\int \frac{\mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3} e v^i g_0 = \int \frac{\mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3} e \frac{\partial \epsilon(\boldsymbol{k})}{\partial k_i} g_0(\epsilon) = \int \frac{\mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3} e \frac{\partial G_0[\epsilon(\boldsymbol{k})]}{\partial k_i} = 0$$

where $\partial G(\epsilon)/\partial \epsilon = g_0(\epsilon)$.

$$J^i = \int \frac{\mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3} e \dot{x}^i g = \int \frac{\mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3} \Big[-\frac{e^2}{\hbar} \tilde{b}_{ij} g_0 + \tau e^2 v^j v^i \frac{\partial g_0}{\partial \epsilon} \Big] E_j$$

- **Conductivity**:

$$\sigma_{ij} = \int \frac{\mathrm{d}^3 \boldsymbol{k}}{(2\pi)^3} \Big[-\frac{e^2}{\hbar} \tilde{b}_{ij} g_0 + \tau e^2 v^j v^i \frac{\partial g_0}{\partial \epsilon} \Big]$$

Quantized Hall conductance in 2D

For a filled band, $g_0 = 1$

$$\sigma^H_{ij} = -\int \frac{\mathrm{d}^2\boldsymbol{k}}{(2\pi)^2}\frac{e^2}{\hbar}\tilde{b}_{ij}g_0 = -\epsilon_{ij}n_{\text{Chern}}\frac{e^2}{h}$$

Thouless

where (let $\tilde{b}_{ij} = \epsilon_{ij}\tilde{b}$)

$$n_{\text{Chern}} = \int_{B.Z.}\frac{\mathrm{d}^2k}{2\pi}\tilde{b} = \int_{B.Z.}\frac{\mathrm{d}^2k}{2\pi}\Big(\frac{\partial\tilde{a}_x}{\partial k_y} - \frac{\partial\tilde{a}_y}{\partial k_x}\Big) = \text{integer},$$

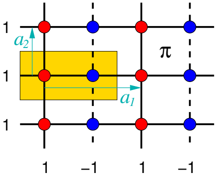
$$\mathrm{i}\,\tilde{a}_i = \langle\psi(\boldsymbol{k})|\partial_{k_i}|\psi(\boldsymbol{k})\rangle.$$

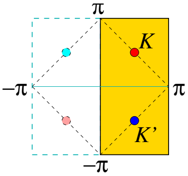
We see that we have a quantized Hall conductance. n_{Chern} is Chern number.

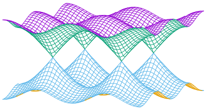
We have a Chern insulator if the total Chern number of the filled bands is non-zero.

- How to make a Chern insulator?

π-flux, Dirac fermion, and its geometric connection $\tilde{\boldsymbol{a}}(\boldsymbol{k})$



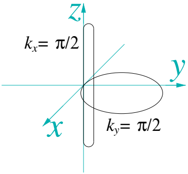




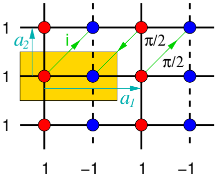
Hopping matrix in $\boldsymbol{k}$-space ($\boldsymbol{a}_1 = 2\boldsymbol{x}$, $\quad \boldsymbol{a}_2 = \boldsymbol{y}$):

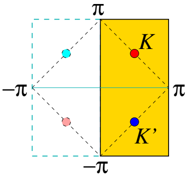
$$M(\boldsymbol{k}) = \begin{pmatrix} 2t\cos(\boldsymbol{a}_2\cdot\boldsymbol{k}) & t + t\,\mathrm{e}^{-\mathrm{i}\,\boldsymbol{a}_1\cdot\boldsymbol{k}} \\ t + t\,\mathrm{e}^{\mathrm{i}\,\boldsymbol{a}_1\cdot\boldsymbol{k}} & -2t\cos(\boldsymbol{a}_2\cdot\boldsymbol{k}) \end{pmatrix} = \begin{pmatrix} 2t\cos k_y & t + t\,\mathrm{e}^{-2\mathrm{i}\,k_x} \\ t + t\,\mathrm{e}^{2\mathrm{i}\,k_x} & -2t\cos k_y \end{pmatrix}$$

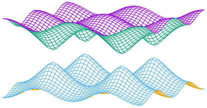
- $M(k) = \boldsymbol{v}(\boldsymbol{k})\cdot\boldsymbol{\sigma}$: $\epsilon = \pm|\boldsymbol{v}(\boldsymbol{k})|$. The vector field $\boldsymbol{v}(\boldsymbol{k})$ on B.Z.:
  $v_x = t + t\cos(2k_x), \qquad v_y = t\sin(2k_x), \qquad v_z = 2t\cos(k_y)$.
  $|\boldsymbol{v}| = t\sqrt{2 + 2\cos(2k_x) + 4\cos^2(k_y)} = t\sqrt{4\cos^2(k_x) + 4\cos^2(k_y)}$.
- Eigenstate in conduction band $|\boldsymbol{n}(\boldsymbol{k})\rangle$,
  $\boldsymbol{n}(\boldsymbol{k}) = \boldsymbol{v}(\boldsymbol{k})/|\boldsymbol{v}(\boldsymbol{k})|$, has geometric connection
  $\mathrm{i}\,\tilde{a}_i(\boldsymbol{k}) = \langle \boldsymbol{n}(\boldsymbol{k})|\partial_{k_i}|\boldsymbol{n}(\boldsymbol{k})\rangle$: $\tilde{b}_{xy} = \partial_{k_x}\tilde{a}_y - \partial_{k_y}\tilde{a}_x \neq 0$
  $\oint_K \mathrm{d}\boldsymbol{k}\cdot\tilde{\boldsymbol{a}} = \pi$, $\oint_{K'} \mathrm{d}\boldsymbol{k}\cdot\tilde{\boldsymbol{a}} = \pi$ → two π-flux tubes.



$\pi/2$-flux state: complex hopping $\to$ Chern insulator



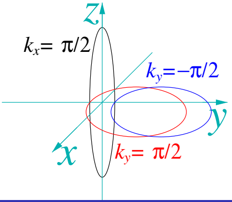




Hopping matrix in $\boldsymbol{k}$-space ($\boldsymbol{a}_1 = 2\boldsymbol{x}$, $\quad \boldsymbol{a}_2 = \boldsymbol{y}$): $M(\boldsymbol{k}) =$

$$\begin{pmatrix} 2t\cos(\boldsymbol{a}_2\cdot\boldsymbol{k}) & t + t\,e^{-i\,\boldsymbol{a}_1\cdot\boldsymbol{k}} + i\,t'\,e^{i\,\boldsymbol{a}_2\cdot\boldsymbol{k}} + i\,t'\,e^{-i\,(\boldsymbol{a}_2\cdot\boldsymbol{k}+\boldsymbol{a}_1\cdot\boldsymbol{k})} \\ t + t\,e^{i\,\boldsymbol{a}_1\cdot\boldsymbol{k}} - i\,t'\,e^{-i\,\boldsymbol{a}_2\cdot\boldsymbol{k}} - i\,t'\,e^{i\,(\boldsymbol{a}_2\cdot\boldsymbol{k}+\boldsymbol{a}_1\cdot\boldsymbol{k})} & -2t\cos(\boldsymbol{a}_2\cdot\boldsymbol{k}) \end{pmatrix}$$

- $M(k) = \boldsymbol{v}(\boldsymbol{k})\cdot\boldsymbol{\sigma}$: $\epsilon = \pm|\boldsymbol{v}(\boldsymbol{k})|$. The vector field $\boldsymbol{v}(\boldsymbol{k})$ on B.Z.:
  $v_x = t + t\cos(2k_x) - t'\sin(k_y) + t'\sin(k_y + 2k_x)$,
  $v_y = t\sin(2k_x) - t'\cos(k_y) - t'\cos(k_y + 2k_x)$, $v_z = 2t\cos(k_y)$.
- Eigenstate in conduction band $|\boldsymbol{n}(\boldsymbol{k})\rangle$,
  $\boldsymbol{n}(\boldsymbol{k}) = \boldsymbol{v}(\boldsymbol{k})/|\boldsymbol{v}(\boldsymbol{k})|$, has geometric connection
  $i\,\tilde{a}_i(\boldsymbol{k}) = \langle \boldsymbol{n}(\boldsymbol{k})|\partial_{k_i}|\boldsymbol{n}(\boldsymbol{k})\rangle$: $\tilde{b}_{xy} = \partial_{k_x}\tilde{a}_y - \partial_{k_y}\tilde{a}_x \neq 0$
  $\to$ The wrapping number (Chern number) $= 1$

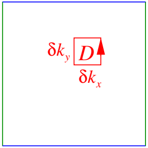


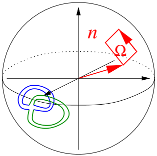
Chern insulator (IQH state)

Geometric phase from geometric connection $\tilde{\boldsymbol{a}}(\boldsymbol{k})$

- Geometric phase $\phi = \oint_{\partial D} \mathrm{d}\boldsymbol{k} \cdot \tilde{\boldsymbol{a}}(\boldsymbol{k}) = \frac{1}{2}\Omega$

$$\phi = \oint_{\partial B.Z.} \mathrm{d}\boldsymbol{k} \cdot \tilde{\boldsymbol{a}}(\boldsymbol{k}) = 2\pi \times \text{wraping num.}$$





- Geometric curvature $\tilde{B} = \partial_{k_x}\tilde{a}_y - \partial_{k_y}\tilde{a}_x$.

$$\phi = \oint_{\partial D} \mathrm{d}\boldsymbol{k} \cdot \tilde{\boldsymbol{a}}(\boldsymbol{k}) = \int_D \mathrm{d}^2 k \tilde{B},$$

$$\int_{B.Z.} \mathrm{d}^2 k \tilde{B} = 2\pi \times \text{Chern number}$$

- Compute geometric curvature:

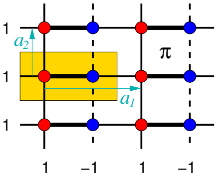
$$\tilde{B}\delta k_x \delta k_y = \tfrac{1}{2}\boldsymbol{n} \cdot \Big([\boldsymbol{n}(\boldsymbol{k} + \delta k_x \boldsymbol{x}) - \boldsymbol{n}(\boldsymbol{k})] \times [\boldsymbol{n}(\boldsymbol{k} + \delta k_y \boldsymbol{y}) - \boldsymbol{n}(\boldsymbol{k})] \Big)$$

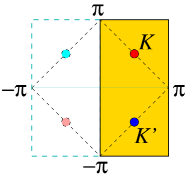
$$\tilde{B}(\boldsymbol{k}) = \frac{1}{2}\boldsymbol{n} \cdot [\partial_{k_x}\boldsymbol{n}(\boldsymbol{k}) \times \partial_{k_y}\boldsymbol{n}(\boldsymbol{k})]$$

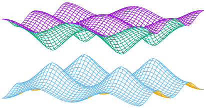
- Compute Chern number (the wrapping number):

$$(4\pi)^{-1} \int_{B.Z.} \mathrm{d}^2 k \ \boldsymbol{n} \cdot [\partial_{k_x}\boldsymbol{n}(\boldsymbol{k}) \times \partial_{k_y}\boldsymbol{n}(\boldsymbol{k})] = \text{Chern number}$$

Dimmer state





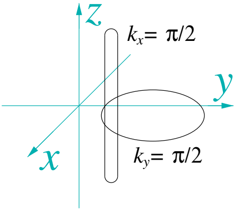


Hopping matrix in $\boldsymbol{k}$-space ($\boldsymbol{a}_1 = 2\boldsymbol{x}, \quad \boldsymbol{a}_2 = \boldsymbol{y}$):

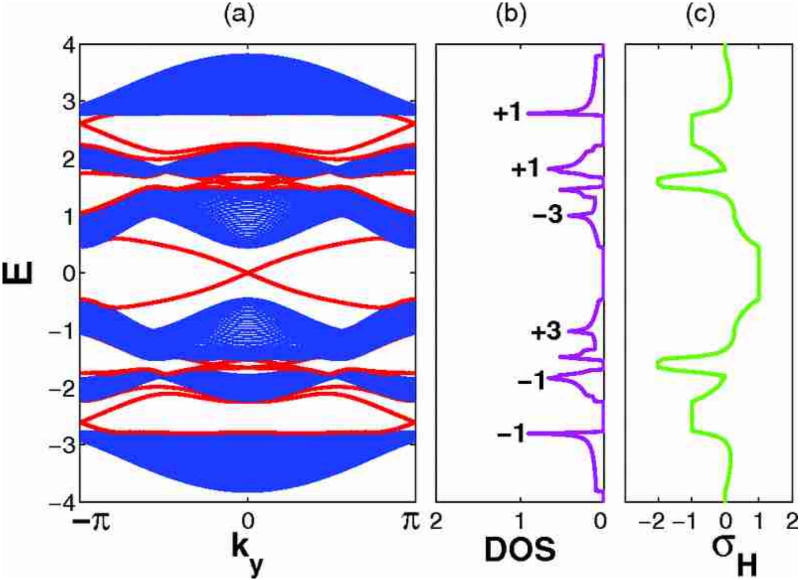
$$M(\boldsymbol{k}) = \begin{pmatrix} 2t\cos(\boldsymbol{a}_2 \cdot \boldsymbol{k}) & t' + t\,\mathrm{e}^{-\mathrm{i}\,\boldsymbol{a}_1 \cdot \boldsymbol{k}} \\ t' + t\,\mathrm{e}^{\mathrm{i}\,\boldsymbol{a}_1 \cdot \boldsymbol{k}} & -2t\cos(\boldsymbol{a}_2 \cdot \boldsymbol{k}) \end{pmatrix}$$

- $M(k) = \boldsymbol{v}(\boldsymbol{k}) \cdot \boldsymbol{\sigma}$: $\epsilon = \pm|\boldsymbol{v}(\boldsymbol{k})|$. The vector field $\boldsymbol{v}(\boldsymbol{k})$ on B.Z.:
  $v_x = t' + t\cos(2k_x), \qquad v_y = t\sin(2k_x), \qquad v_z = 2t\cos(k_y)$.
- Eigenstate in conduction band $|\boldsymbol{n}(\boldsymbol{k})\rangle$,
  $\boldsymbol{n}(\boldsymbol{k}) = \boldsymbol{v}(\boldsymbol{k})/|\boldsymbol{v}(\boldsymbol{k})|$, has geometric connection
  $\mathrm{i}\,\tilde{a}_i(\boldsymbol{k}) = \langle \boldsymbol{n}(\boldsymbol{k})|\partial_{k_i}|\boldsymbol{n}(\boldsymbol{k})\rangle$: $\tilde{b}_{xy} = \partial_{k_x}\tilde{a}_y - \partial_{k_y}\tilde{a}_x \neq 0$
  $\to$ The wrapping number (Chern number) $= 0$

  Atomic insulator



Chern number of the bands



Continuum limit and Dirac equation (Dirac fermion)

- Near K-point $(\frac{\pi}{2}, \frac{\pi}{2})$

$$M(\delta \boldsymbol{k} + K) = -2t\delta k_x \sigma^y - 2t\delta k_y \sigma^z + \Delta_K \sigma^x$$

  The $\boldsymbol{k}$-space magnetic field $\tilde{b}_{xy}$ has a peak near K-point with total flux π. The sign of $\tilde{b}_{xy}$ is determined by the handness of $(-2t\sigma^y, -2t\sigma^z, \Delta_K \sigma^x)$

- $\boldsymbol{k}$-space Shrödinger equation: $\mathrm{i}\hbar\dot{\psi}_{\delta\boldsymbol{k}} = M(\delta\boldsymbol{k} + K)\psi_{\delta\boldsymbol{k}}$
  $\boldsymbol{x}$-space Shrödinger equation ($\delta\boldsymbol{k} \to -\mathrm{i}\boldsymbol{\partial}$):

$$\mathrm{i}\hbar\dot{\psi}(\boldsymbol{x}) = 2\mathrm{i}t(\sigma^y\partial_x + \sigma^z\partial_y + \Delta_K\sigma^x)\psi(\boldsymbol{x})$$

  Dirac equation (multiply σ^x on both sides):

$$(\mathrm{i}\hbar\sigma^x\partial_t + 2t\sigma^z\partial_x - 2t\sigma^y\partial_y + \Delta_K)\psi(\boldsymbol{x}) = 0$$
$$(\gamma_K^t\partial_t + v\gamma_K^x\partial_x + v\gamma_K^y\partial_y + \hbar^{-1}\Delta_K)\psi(\boldsymbol{x}) = 0$$
$$\gamma_K^t = \mathrm{i}\sigma^x,\ \gamma_K^x = \sigma^z,\ \gamma_K^y = -\sigma^y, \quad \{\gamma_K^\mu, \gamma_K^\nu\} = 2\eta^{\mu\nu},\ \mu,\nu = t,x,y.$$

Continuum limit and Dirac equation (Dirac fermion)

- Near K'-point $(\frac{\pi}{2}, \frac{\pi}{2})$

$$M(\delta \boldsymbol{k} + K') = -2t\delta k_x \sigma^y + 2t\delta k_y \sigma^z + \Delta_{K'}\sigma^x$$

  The $\boldsymbol{k}$-space magnetic field $\tilde{b}_{xy}$ has a peak near K-point with total flux π. The sign of $\tilde{b}_{xy}$ is determined by the handness of $(-2t\sigma^y, 2t\sigma^z, \Delta_{K'}\sigma^x)$

- Dirac equation:

$$(\gamma^t_{K'}\partial_t + v\gamma^x_{K'}\partial_x + v\gamma^y_{K'}\partial_y + \hbar^{-1}\Delta_{K'})\psi(\boldsymbol{x}) = 0$$

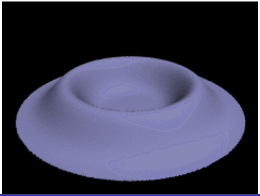
$$\gamma^t_{K'} = \mathrm{i}\sigma^x,\ \gamma^x_{K'} = \sigma^z,\ \gamma^y_{K'} = \sigma^y, \quad \{\gamma^\mu_{K'}, \gamma^\nu_{K'}\} = 2\eta^{\mu\nu},\ \mu,\nu = t,x,y.$$

- For the dimmer phase $\Delta_K = \Delta_{K'}$. The handness of $(-2t\sigma^y, -2t\sigma^z, \Delta_K\sigma^x)$ and $(-2t\sigma^y, 2t\sigma^z, \Delta_{K'}\sigma^x)$ are opposite. The $\boldsymbol{k}$-space flux from K and K' cancel. The Chern number $= 0$.
- For the $\frac{\pi}{2}$-flux phase $\Delta_K = -\Delta_{K'}$. The handness of $(-2t\sigma^y, -2t\sigma^z, \Delta_K\sigma^x)$ and $(-2t\sigma^y, 2t\sigma^z, \Delta_{K'}\sigma^x)$ are the same. The $\boldsymbol{k}$-space flux from K and K' add up to 2π.
  The Chern number $= 1$.

Quantum Hall states and their edge excitations

The $\frac{\pi}{2}$-flux phase (the Chern insulator), although is fully gapped in the bulk, has a gapless boundary which is **topological**. *To see this more easily, we turn off the lattice potential.*

- The Hamiltonian for a 2D electron in a uniform magnetic field B:
$$H = -\sum \frac{1}{2m}(\partial_i - A_i)^2 = -\sum \frac{1}{2m}(\partial_z - \frac{B}{4}z^*)(\partial_{z^*} + \frac{B}{4}z) + const.$$
in complex coordinate $z = x + \mathrm{i}y$ (in $\hbar = c = e = 1$ unit).
- The lowest energy eigenstates: $P(z)\mathrm{e}^{-\frac{1}{4l_B^2}|z|^2}$,
where $P(z) = \sum a_l z^l$, $B = \frac{1}{l_B^2}$, since
$$\mathrm{e}^{\frac{1}{4l_B^2}zz^*}(\mathrm{i}\partial_z - \mathrm{i}\frac{B}{4}z^*)(\mathrm{i}\partial_{z^*} + \mathrm{i}\frac{B}{4}z)\mathrm{e}^{-\frac{1}{4l_B^2}zz^*} = (\mathrm{i}\partial_z - \mathrm{i}\frac{B}{2}z^*)\mathrm{i}\partial_{z^*}$$
- Basis of first Landau level states:
angular momentum l-orbital $z^l\mathrm{e}^{-\frac{1}{4l_B^2}|z|^2}$
with a ring shape with $R_l = \sqrt{2l_B^2 l}$
that enclose l-unit of magnetic flux,
since $\pi R_l^2 B = 2\pi l$.

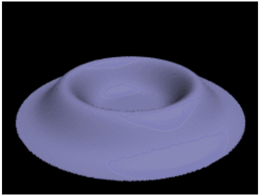
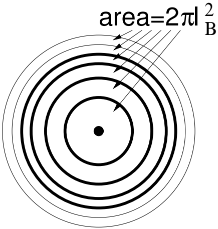


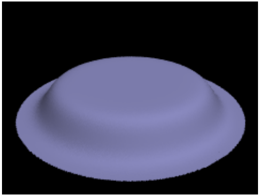
Integer quantum Hall (IQH) state

- Many-body wave function of the IQH state

$$\Psi = P_1(z_1, \cdots, z_N)\mathrm{e}^{-\frac{1}{4l_B^2}\sum_{i=1}^N z_i z_i^*}, \qquad P_1 = \prod_{i<j}(z_i - z_j).$$

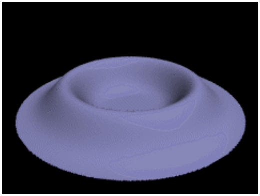
- Let S_N is the power of z's in $P(z_1, \cdots, z_N)$, the total angular momentum of the N-electron state: $S_N = \frac{N(N-1)}{2}$
- Let $l_N = S_N - S_{N-1}$ $\to$ the N^{th} electron is added to the angular momentum l_N-orbital: $l_N = N - 1$
- The shape of quantum Hall wave function

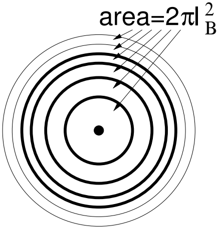



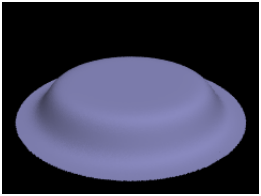


$\to$ P_1 is a filling fraction $\nu = 1$ IQH state.

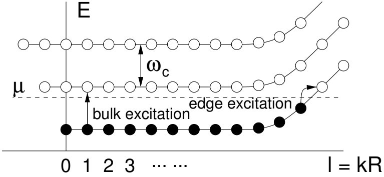
Edge excitations of IQH state: chiral edge

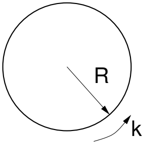






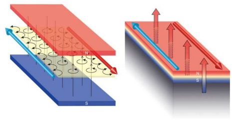
In the presence of circular confining potential, the angular momentum l-orbital has a non-zero energy $E(l)$. Since $l = kR$ (R = radius of the droplet), edge electron dispersion relation $\epsilon(k) = E(kR)$. The velocity of edge excitation is $v = c|\boldsymbol{E}|/|\boldsymbol{B}|$.

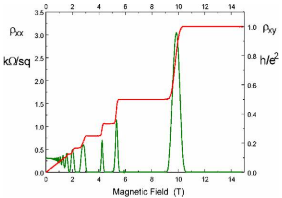


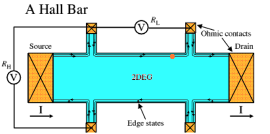


All excitations on the edge move in the same direction.

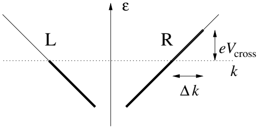
Physics of chiral edge states: Quantized Hall effect





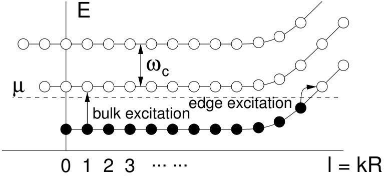


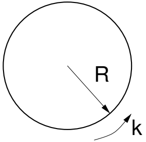
- $I = ev_{\text{edge}}\Delta n_{1D} = ev_{\text{edge}}\Delta k/2\pi = e\frac{eV_{\text{cross}}}{\hbar}$
  $= \frac{e^2}{h}V_{\text{cross}} \to \sigma_{xy} = \frac{I}{V_{\text{cross}}} = \frac{e^2}{h}$.



- Wrapping number of the band
  $=$ number of edge modes $\to$

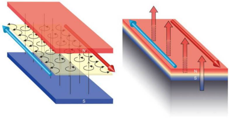
$\sigma_{xy} = \frac{I}{V_{\text{cross}}} =$ Wrapping-number $\times \frac{e^2}{h} =$ Chern-number $\times \frac{e^2}{h}$.

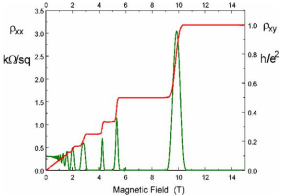


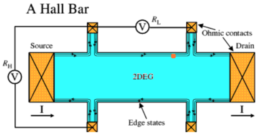


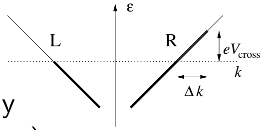
von Klitzing

Physics of chiral edge states: Perfect conducting channel



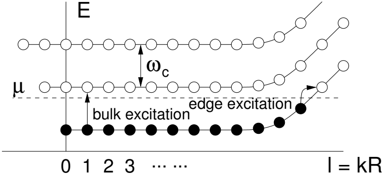


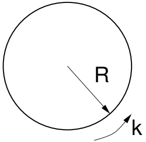




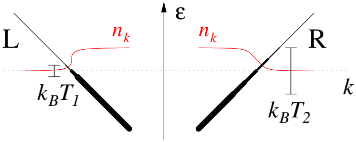
- Electrons on one edge cannot turn back, have to go forward $\to$ $V_{\text{drop}} = 0, \quad R_{xx} = 0$
- The non-zero voltage drop $V_{\text{drop}} \neq 0$ can only come from interedge tunneling (back scattering):

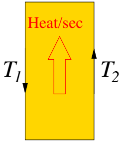
$$V_{\text{drop}} \sim \mathrm{e}^{-\Delta\epsilon/k_B T}$$





Universal thermal Hall conductance κ





- Heat flux $= \kappa \Delta T$. Heat flux $=$ entropy flux $\times$ T
- Entropy for one electron $S = -k_B n_k \log n_k$. $n_k = \frac{1}{e^{\epsilon_k/k_B T}+1}$.
- Entropy density

$$s = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} (-k_B n_k \log n_k) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} k_B \frac{\log(e^{\epsilon_k/k_B T}+1)}{e^{\epsilon_k/k_B T}+1}$$

- Heat flux $= \int_{-\infty}^{+\infty} \frac{dk}{2\pi} v T k_B \frac{\log(e^{\hbar v k/k_B T}+1)}{e^{\hbar v k/k_B T}+1} = \frac{(k_B T)^2}{\hbar} \int_{-\infty}^{+\infty} \frac{dx}{2\pi} \frac{\log(e^x+1)}{e^x+1}$

$$\int dx \frac{\log(e^x+1)}{e^x+1} = \frac{\pi^2}{6}$$

Heat flux $= \frac{(k_B T)^2 \pi}{12\hbar}$, Total heat flux $= \frac{k_B^2 \pi}{12\hbar}(T_2^2 - T_1^2) = \frac{\pi k_B^2 T}{6\hbar} \Delta T$

- Thermal Hall conductance $\kappa = \frac{\pi}{6} \frac{k_B^2 T}{\hbar}$
- In general $\kappa = c \frac{\pi}{6} \frac{k_B^2 T}{\hbar}$, $c = \#$ of right-modes $- \#$ of left-modes

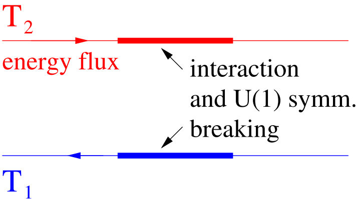
Stability of Chern insulator against $U(1)$ symm. breaking

- **Chern insulator**: non-interacting fermions with translation and $U(1)$ symmetry, characterized by the non-zero Chern number of the filled band in the Brillouin zone.
- If we break the $U(1)$ symmetry (by attaching a superconductor), there will be no Hall conductance nor $U(1)$-Chern-Simons term. *Is Chern insulator still well defined, ie still different from the trivial insulator?*

Robust $c = 1$ chiral gapless edge state

- The thermal Hall conductance $\kappa = \frac{\pi}{6}\frac{k_B^2 T}{\hbar}$ is always quantized, *since the time-independent interaction and $U(1)$-symmetry breaking terms cannot change the energy flux, and the energy flux cannot flow backwards and cross the bulk.*

  The 2D topological phase for fermions



- The thermal Hall conductance $\kappa = \frac{\pi}{6}\frac{k_B^2 T}{\hbar}$ is robust against $U(1)$ symm. breaking and interaction. $\to$ Chern insulator (IQH state) is robust against $U(1)$ symm. breaking and interaction, although it is constructed for non-interacting fermions with $U(1)$ symm.

  Chern insulator (IQH state) has a non-trivial topological order (*ie* cannot smoothly deform into trivial insulator via any paths that can have interaction and break any symmetries)

Summary: a more general example

- n layers of $N_{\text{Chern}} = 1$ Chern insulators of charge-1 fermions
  $+$ m layers of $N_{\text{Chern}} = -1$ Chern insulators of charge-0 fermions.
- Hall conductance $\sigma_{xy} = \frac{n}{2\pi}$.
  Thermal Hall conductance $\kappa = (n-m)\frac{\pi}{6}\frac{k_B^2 T}{\hbar}$
  (*ie* chiral central charge $c = n - m$).
- **Different phases of 2D gapped fermion systems without any symmetry and with non-degenerate ground state on torus are labeled by (at least) one integer $c = n - m$.**
  Non-zero c $\rightarrow$ non-trivial topological order (Cannot be deformed into product state)
- **Different phases of 2D gapped fermion systems with $U(1)$ symmetry and non-degenerate ground state on torus are labeled by (at least) two integers (n, m).**
  $\rightarrow$ symmetry enriched topological order (Cannot be deformed into product state if we break the symmetry. Cannot be deformed into each other if we preserve the symmetry.)