Modern quantum many-body physics – Semi-classical approach

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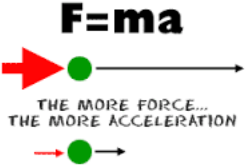
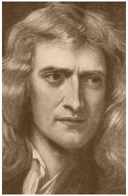
Classical motion of a particle and Newton's Law

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:

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

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 $\mathcal{V}$:

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

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

- Phase-space Lagrangian (taking $\hbar = 1$ unit)

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

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

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

we get the equation of motion

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

Quantum $\to$ classical: 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 $\to$ 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

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

where

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

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

Most general phase-space description of classical system

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

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

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

and the equation of motion

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

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

- Choose an equivalent (redundant) trial wave function $\mathrm{e}^{\mathrm{i}\theta(\xi^I)}|\psi_{\xi^I}\rangle$:

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

which gives rise to the same EOM. Phase space Lagrangian is a way to lable/describe a physical system. **Two phase space Lagrangians, differing by a total time derivative of any function, label/describe the same system → Gauge redundancy**

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

Differential form

- The phase space "vector potential" a_I gives rise to a differential 1-form, $a = a_I \mathrm{d}\xi^I$.
  The phase space "magnetic field" b_{IJ} gives rise to a differential 2-form, $b = b_{IJ} \mathrm{d}\xi^I \wedge \mathrm{d}\xi^J/2!$ (assuming the sum of indices), where $\wedge$ is the **wedge product** $\mathrm{d}\xi^I \wedge \mathrm{d}\xi^J = -\mathrm{d}\xi^J \wedge \mathrm{d}\xi^I$.
- The physical meaning of the 2-form: for any 2-dimensional submanifold $M^2 \subset M_{\text{phase space}}$, the pair $b,\ M^2$ give rise to a number:
  $$\langle b, M^2\rangle = \int_{M^2} b = \int_{M^2} b_{IJ} \mathrm{d}\xi^I \mathrm{d}\xi^J/2! = \int_{M^2} b_{xy} \mathrm{d}x \mathrm{d}y = \text{number} = \text{flux}.$$
  which is called **evaluate 2-form b on 2-manifold M^2.**
  So the 2-form b describes a "magnetic field" in the phase space $M_{\text{phase space}}$.
- n-form: $\omega_n = \omega_{I_1 \dots I_n} \mathrm{d}\xi^{I_1} \wedge \cdots \wedge \mathrm{d}\xi^{I_n}/n!$
  Evaluate n-form ω_n on n-manifold M^n: $\langle \omega_n, M^n\rangle = \int_{M^n} \omega_n = \text{number}$
- For a m-form and a n-form, we have $\omega_m \wedge \omega_n = (-)^{m+n} \omega_n \wedge \omega_m$.

Generalized Stokes theorem in differential form

- **Exterior derivative** d maps a n-form to a $n+1$-form: $\omega_n \to \nu_{n+1}$

  $\nu_{n+1} \equiv \mathrm{d}\omega_n = (\partial_{I_0}\omega_{I_1\cdots I_n})\mathrm{d}\xi^{I_0}\wedge\cdots\wedge\mathrm{d}\xi^{I_n}/(n+1)!$ (with sum of indices)

  $\nu_{n+1} = \nu_{I_0\cdots I_n}\mathrm{d}\xi^{I_0}\wedge\cdots\wedge\mathrm{d}\xi^{I_n}/(n+1)!,$

  $\nu_{I_0\cdots I_n} = \left(\partial_{I_0}\omega_{I_1\cdots I_n} - \partial_{I_1}\omega_{I_0\cdots I_n} \pm \cdots\right)_{\text{anti-symmetrize}}/(n+1)!$

- $b_{IJ} = \partial_I a_J - \partial_J a_I \to b = (\partial_I a_J - \partial_J a_I)\mathrm{d}\xi^I\mathrm{d}\xi^J/2! = \partial_I a_J \mathrm{d}\xi^I\mathrm{d}\xi^J = \mathrm{d}a$.
- $\mathrm{d}\omega_n\nu_m = (\mathrm{d}\omega_n)\nu_m + (-)^n\omega_n(\mathrm{d}\nu_m)$.

- Generalized Stokes theorem
$$\int_{M^{n+1}} \mathrm{d}\omega_n = \int_{\partial M^{n+1}} \omega_n$$

- **Definition**: ω_n is **closed** if $\mathrm{d}\omega_n = 0$.
  Definition: ω_n is **exact** there is a $n-1$-form μ_{n-1} such that $\omega_n = \mathrm{d}\nu_{n-1}$. Since $\mathrm{d}\mathrm{d} = 0$, an exact form is also a closed form.
- Two vector potential 1-forms differing by an exact 1-from are equivalent

- ω_n is exact iff $\int_{M^n}\omega_n = 0$ for any closed manifold M^n. ω_n is closed iff $\int_{M^n}\omega_n = 0$ for any contractible closed manifold M^n.

- **A magnetic field is described by a closed (or exact?) 2-form b.**

Generalized Liouville's theorm

- **Generalized Liouville's theorem**
  Consider a time evolution from $t \to \tilde{t}$, $\xi^I \to \tilde{\xi}^I$, determined by the equation of motion
  $$b_{IJ}\dot{\xi}^J = -\frac{\partial \bar{H}}{\partial \xi^I}$$
  Then $\mathrm{Pf}(b_{IJ}(\xi^I))\mathrm{d}^n\xi^I = \mathrm{Pf}(b_{IJ}(\tilde{\xi}^I))\mathrm{d}^n\tilde{\xi}^I \quad (b_{xp}\mathrm{d}x\,\mathrm{d}p = b_{\tilde{x}\tilde{p}}\mathrm{d}\tilde{x}\,\mathrm{d}\tilde{p})$

  In other words, the **sympletic volume** $\mathrm{Pf}(b_{IJ}(\xi^I))\mathrm{d}^n\xi^I$ is invariant under time evolution.

- The phase space is a **sympletic manifold** characterized by anti-symmetric tensor b_{IJ}: area element $\mathrm{d}S^2 = b_{IJ}\mathrm{d}\xi^I \wedge \mathrm{d}\xi^J/2!$.
- It is different from the usual manifold characterized by symmetric matrics tensor g_{IJ}: distance^2 element $\mathrm{d}s^2 = g_{IJ}\mathrm{d}\xi^I \cdot \mathrm{d}\xi^J$.

- **A classical system is described by pair $\big(M_{\text{phase space}}, H(\xi^I)\big)$, a sympletic manifold and a function (Hamiltonian) on it.**

Change of variables

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

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

where

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

$$b^\eta_{IJ} = \partial_{\eta^I}(\underbrace{a_K \frac{\partial \xi^K}{\partial \eta^J}}_{a^\eta_J}) - \partial_{\eta^J}(\underbrace{a_K \frac{\partial \xi^K}{\partial \eta^I}}_{a^\eta_I}) = (\partial_{\eta^I} a_K)\frac{\partial \xi^K}{\partial \eta^J} - (\partial_{\eta^J} a_K)\frac{\partial \xi^K}{\partial \eta^I}$$

$$= (\partial_{\xi^L} a_K)\frac{\partial \xi^L}{\partial \eta^I}\frac{\partial \xi^K}{\partial \eta^J} - \underbrace{(\partial_{\xi^L} a_K)\frac{\partial \xi^L}{\partial \eta^J}\frac{\partial \xi^K}{\partial \eta^I}}_{\text{exchange } K\leftrightarrow L} = (\partial_{\xi^L} a_K - \partial_{\xi^K} a_L)\frac{\partial \xi^L}{\partial \eta^I}\frac{\partial \xi^K}{\partial \eta^J}$$

$$= b_{LK}\frac{\partial \xi^L}{\partial \eta^I}\frac{\partial \xi^K}{\partial \eta^J}. \qquad b^\eta_{IJ}\,\mathrm{d}\eta^I\,\mathrm{d}\eta^J = b_{IJ}\,\mathrm{d}\xi^I\,\mathrm{d}\xi^J.$$

Derive generalized Liouville's theorm

- For the time evolution from $t \to \tilde t$, $\xi^I \to \tilde\xi^I$, we have

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

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

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

- Assume for η^I variable, b^η_{IJ} is indenpendent of η^I. Then, $\partial_I(b^{IK}) = 0$ and $\mathrm{Det}(\hat J) = 1$. We have the **Liouville's theorm**

$$\mathrm{d}^n\eta^I = \mathrm{d}^n\tilde\eta^I \text{ or } \sqrt{\mathrm{Det}(b^\eta_{IJ}(\eta^I))}\mathrm{d}^n\eta^I = \sqrt{\mathrm{Det}(b^\eta_{IJ}(\tilde\eta^I))}\mathrm{d}^n\tilde\eta^I \ (b^\eta \text{ ind. of } \eta^I)$$

- Change variables $\to$ **Generalized Liouville's theorem**

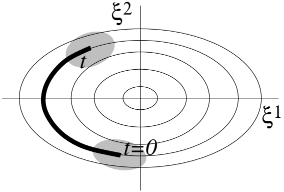
$$\sqrt{\mathrm{Det}(b^\eta_{IJ})}\mathrm{Det}(\frac{\partial\eta^I}{\partial\xi^J})\mathrm{Det}(\frac{\partial\xi^I}{\partial\eta^J})\mathrm{d}^n\eta^I = \sqrt{\mathrm{Det}(\tilde b^\eta_{IJ})}\mathrm{Det}(\frac{\partial\tilde\eta^I}{\partial\tilde\xi^J})\mathrm{Det}(\frac{\partial\tilde\xi^I}{\partial\tilde\eta^J})\mathrm{d}^n\tilde\eta^I$$

$$\sqrt{\mathrm{Det}(b_{IJ}(\xi^I))}\mathrm{d}^n\xi^I = \sqrt{\mathrm{Det}(b_{IJ}(\tilde\xi^I))}\mathrm{d}^n\tilde\xi^I$$

$$\to \qquad \mathrm{Pf}(b_{IJ}(\xi^I))\mathrm{d}^n\xi^I = \mathrm{Pf}(b_{IJ}(\tilde\xi^I))\mathrm{d}^n\tilde\xi^I$$

Phase-space volume occupied by a quantum state

- For a classical theory every phase-space 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.



- *How many quantum states does a phase space region D^n contain?* From the generalized Liouville's theorm and conservation of degrees of freedom, 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.

Density of quantum states and the sympletic structure

- The number of quantum state in a region D^n in n-dimensional phase space can also be written in term of diferetial 2-form, $b = b_{IJ}\,\mathrm{d}\xi^I\,\mathrm{d}\xi^J/2!$, that defines the sympletic structure of the phase space:

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

Example: For 2-dimensional phase space

$$\int_{D^2} \frac{b}{(2\pi)} = \int_{D^2} \frac{b_{IJ}\,\mathrm{d}\xi^I\,\mathrm{d}\xi^J/2!}{2\pi} = \int_{D^2} \frac{b_{12}\,\mathrm{d}\xi^1\,\mathrm{d}\xi^2}{2\pi}$$

The number of quantum state in the region D^2 is equal to the number of flux quantum (also called **Chern number**) through D^2 for the phase space "magnetic" field b_{IJ}.

- **Quantization of "magnetic" field**: If D^n is closed (*ie* is the whole phase space)

$$\int_{D^n} \frac{b^{n/2}}{(2\pi)^{n/2}} \in \mathbb{Z} \qquad \text{(higher Chern number)}$$

An example: an anharmonic oscillator

- What is low energy spectrum of

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

- 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

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

- 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 in a phase space region D^2

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

which is what we expected.

An anharmonic oscillator

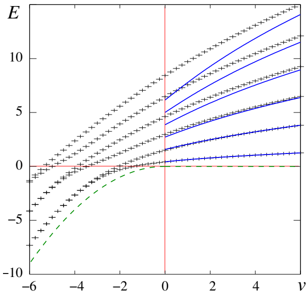
- The small motions around the ground state ξ_0^I $\to$ A collection of Harmonic oscillators $\to$ low energy spectrum.

- 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 $\omega = \sqrt{v\big(1 + \frac{3}{2\alpha v}\big)}$.



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

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

Geometric phase and related mathematics

$\delta\phi = a_I \mathrm{d}\xi^I = -\mathrm{i}\langle\psi_{\xi^I}|\frac{\partial}{\partial\xi^I}|\psi_{\xi^I}\rangle \mathrm{d}\xi^I$ is the so call **geometric phase**.

- *What is the geometric phase?*
  Consider $|\psi_{\xi^I}\rangle$ and $|\psi_{\xi^I+\delta\xi^I}\rangle$, what is the phase difference 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 differnce cannot be characterized by a phase.
- But for small $\delta\xi^I$, the leading difference is just a phase factor

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

since, to the first order in δ

$$\begin{aligned} 0 &= \delta\langle\psi_{\xi^I}|\psi_{\xi^I}\rangle = (\langle\psi_{\xi^I+\delta\xi^I}| - \langle\psi_{\xi^I}|)|\psi_{\xi^I}\rangle + \langle\psi_{\xi^I}|(|\psi_{\xi^I+\delta\xi^I}\rangle - |\psi_{\xi^I}\rangle) \\ &= [\langle\psi_{\xi^I+\delta\xi^I}|\psi_{\xi^I}\rangle - 1] + [\langle\psi_{\xi^I}|\psi_{\xi^I+\delta\xi^I}\rangle - 1] \to [\langle\psi_{\xi^I+\delta\xi^I}|\psi_{\xi^I}\rangle - 1] = \text{imag} \end{aligned}$$

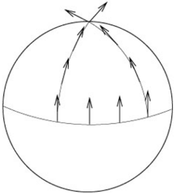
Therefore $\langle\psi_{\xi^I}|\psi_{\xi^I+\delta\xi^I}\rangle \approx \mathrm{e}^{\mathrm{i}\,O(\delta\xi)}$, or

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

Is the geometric phase meaningless?

- Geometric phase $e^{i\delta\phi} = \langle\psi_{\xi^I}|\psi_{\xi^I+\delta\xi^I}\rangle = e^{i a_I \delta\xi^I}$. But we can always change the phase of $|\psi_{\xi^I+\delta\xi^I}\rangle \to |\psi_{\xi^I+\delta\xi^I}\rangle_1 = e^{-i a_I \delta\xi^I}|\psi_{\xi^I+\delta\xi^I}\rangle$, to make the geometric phase to be zero: $\langle\psi_{\xi^I}|\psi_{\xi^I+\delta\xi^I}\rangle' = e^{-i a_I \delta\xi^I} e^{i a_I \delta\xi^I} = 1$.

- The move $|\psi_{\xi^I}\rangle \to |\psi_{\xi^I+\delta\xi^I}\rangle$ is a generic transportation.
- The move $|\psi_{\xi^I}\rangle \to |\psi_{\xi^I+\delta\xi^I}\rangle'$ is a **parallel transportation**.
It appears that we can always make geometric phase = 0, and the geometric phase is meaningless. This is wrong!



- As we change the phase of $|\psi_{\xi^I}\rangle$: $|\psi_{\xi^I}\rangle \to e^{i f(\xi^I)}|\psi_{\xi^I}\rangle$, the geometric phase (*ie* the connection) also changes: $a^I \to a^I + \partial_{\xi^I} f$

- We can always choose a f to make $a^I = 0$ along a particular path $\xi^I(t)$, to make $|\psi_{\xi^I(t)}\rangle$ to have the same phase for all t $\to$ parallel transportation along the path.
- But, we cannot find a f to make $a^I = 0$ for all ξ^I, *ie* to make all $|\psi_{\xi^I}\rangle$'s to have the same phase. Some part of geometric phase (or vector potential) a^I is physical, and other part is not. The meaningful part is the "magnetic field": $b_{IJ} = \partial_{\xi^I} a_J - \partial_{\xi^J} a_I$, which is quantized.

What is the geometric phase for spin-1/2?

Consider a spin-$1/2$ state in $\boldsymbol{n}$-direction $|\boldsymbol{n}\rangle = \begin{pmatrix} e^{-i\varphi/2}\cos(\theta/2) \\ e^{i\varphi/2}\sin(\theta/2) \end{pmatrix}$

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

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

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

- $e^{i(a_\theta\delta\theta + a_\varphi\delta\varphi)} = e^{i a_I \delta\xi^I}$ 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.)

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

$$e^{i\sum \delta\varphi(t)} = \langle \boldsymbol{n}(0)|\boldsymbol{n}(t_1)\rangle\langle \boldsymbol{n}(t_1)|\boldsymbol{n}(t_2)\rangle\langle \boldsymbol{n}(t_2)|\boldsymbol{n}(t_3)\rangle \cdots \langle \boldsymbol{n}(t_{N-1})|\boldsymbol{n}(1)\rangle$$
$$= e^{i\sum \boldsymbol{a}(t)\cdot\delta\boldsymbol{n}(t)} = e^{i\int \boldsymbol{a}(t)\cdot d\boldsymbol{n}(t)} = e^{i\int \boldsymbol{a}(t)\cdot \frac{d\boldsymbol{n}(t)}{dt}\, dt}$$

- If we change the phase of $|\boldsymbol{n}\rangle$: $|\boldsymbol{n}\rangle \to e^{if(\boldsymbol{n})}|\boldsymbol{n}\rangle$, the total geometric phase for a loop – the **geometric flux** – does not change.

- Computing the geometric flux:
$\oint_C a_\theta d\theta + a_\varphi d\varphi = \int_D (\partial_\theta a_\varphi - \partial_\varphi a_\theta) d\theta d\varphi$ or $\oint_C a = \int_D da = \int_D b$.
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
$(\theta,\varphi) \to (\theta+\Delta\theta,\varphi) \to (\theta+\Delta\theta,\varphi+\Delta\varphi) \to (\theta,\varphi+\Delta\varphi) \to (\theta,\varphi)$.

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

$|\boldsymbol{n}\rangle = \begin{pmatrix} \cos(\theta/2) \\ \mathrm{e}^{\mathrm{i}\varphi}\sin(\theta/2) \end{pmatrix} \to a_\theta = 0, \quad a_\varphi = \sin(\theta/2)\sin(\theta/2) = \frac{1-\cos(\theta)}{2}$

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

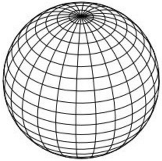
For a loop $(\theta,\varphi) \to (\theta+\Delta\theta,\varphi) \to (\theta+\Delta\theta,\varphi+\Delta\varphi) \to (\theta\theta,\varphi+\Delta\varphi) \to (\theta,\varphi)$:

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

$$= \frac{1}{2}\sin(\theta)\Delta\theta\Delta\varphi = b_{\theta\varphi}\mathrm{d}\theta\,\mathrm{d}\varphi = \frac{1}{2}\Omega([\Delta\theta,\Delta\varphi]) = \text{half solid angle.}$$

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

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



$= 2\pi \times$ Chern number. Spin-1/2 has a Chern number $= 1$

- On shpere the number states = Chern number $+1$.

  On torus the number states = Chern number (Landau levels counting)

The geometric phase of spin-1

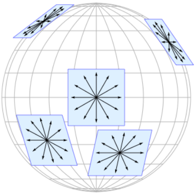
- The geometric connection for spin-1/2 $|\boldsymbol{n}_{S_{\boldsymbol{n}}=\frac{1}{2}}\rangle$ is $(a_\theta^{S=\frac{1}{2}}, a_\varphi^{S=\frac{1}{2}}) = (0, \frac{1-\cos(\theta)}{2})$.
- The geometric connection for spin-1 $|\boldsymbol{n}_{S_{\boldsymbol{n}}=1}\rangle$ is $(a_\theta^{S=1}, a_\varphi^{S=1})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

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

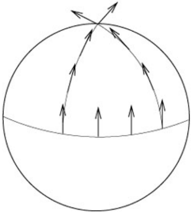
$$\mathrm{e}^{\mathrm{i}\Delta\phi^{S=1}} = \langle \boldsymbol{n}_{S_{\boldsymbol{n}}=1}|\boldsymbol{n}'_{S_{\boldsymbol{n}}=1}\rangle = \langle \boldsymbol{n}_{S_{\boldsymbol{n}}=\frac{1}{2}}|\boldsymbol{n}'_{S_{\boldsymbol{n}}=\frac{1}{2}}\rangle \times \langle \boldsymbol{n}_{S_{\boldsymbol{n}}=\frac{1}{2}}|\boldsymbol{n}'_{S_{\boldsymbol{n}}=\frac{1}{2}}\ra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

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



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 $\to (-\theta,\varphi) = (L_z,\varphi) = (p,x)$ the usual canonical coordinate-momentum pair.

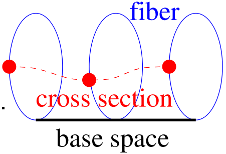
- A particle moving on S^2 with a uniform magnetic field $b_{\theta\varphi}$ of total flux 2π. It is the motion in the lowest Landau level assuming $\hbar\omega_c$ is large. Modified Newton law $\boldsymbol{F} = \boldsymbol{v} \times \boldsymbol{B}$ (not $\boldsymbol{F} = m\boldsymbol{a}$).

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

Lowest Landau level has N_{Chern}-fold degeneracy on a torus.

Global view of geometric phase: S^1 fiber bundle

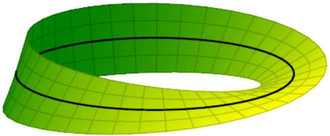
Why the "magnetic field" b is quantuized (*ie* cannot be deformed to 0)?
The physical states are characterized by a point ξ^i on the phase-space, only after we pick the phase of $|\psi(\xi^i)\rangle$. Different choices of phases are equivalent $\to$ the notion of S^1 fiber bundle:



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

- A S^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 S^1 bundle. **Pick a phase = pick a cross section.**

- Trivial S^1 bundle $=$ $S^1 \times$ base-space (globally).
  Non-trivial S^1 fiber bundle has different topology from $S^1 \times$ base-space. No smooth cross section. Trivial and non-trivial bundles describes different classes of classical systems that cannot deform into each other.
- **Vector bundle**: fiber $=$ vector space.
  An example: fiber $= \mathbb{R} \to$ Möbius strip:
  a non-trivial $\mathbb{R}$ bundle on base-space S^1
  No non-zero smooth cross section.



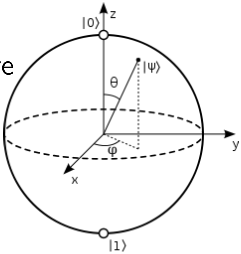
Spin-1/2 example: geometric phase and fiber bundle

- 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 non-trivial **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 one cross section of the fiber bundle $|\boldsymbol{n}\rangle = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\varphi/2}\cos(\theta/2) \\ \mathrm{e}^{\mathrm{i}\varphi/2}\sin(\theta/2) \end{pmatrix}$ or another $|\boldsymbol{n}\rangle = \begin{pmatrix} \cos(\theta/2) \\ \mathrm{e}^{\mathrm{i}\varphi}\sin(\theta/2) \end{pmatrix}$

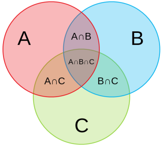
- No smooth cross section $\to$ non-trivial fiber bundle $\neq$ fiber $\times$ base space.

The patch-picture of fiber bundle

The "megnetic field" b in the phase space of a spin is a closed 2-form, but not a exact 2-form, depite $b = \mathrm{d}a$, since the connection 1-form a has singularities on the sphere S^2 (the phase space). There is no continous 1-form a, such that $b = \mathrm{d}a$, since this will imply that

$$\int_{S^2} b = \int_{S^2} \mathrm{d}a = \int_{\partial S^2} a = 0$$

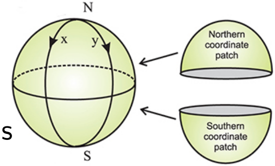
- b **is exact iff the** S^1**-fiber boundle is trivial (*ie* Chern number** $= 0$**)**
- **A fiber boundle is trivial iff it has no continuously defined connection** a **(*ie* the vector potential** a_I**).**



- Any S^1-fiber boundle can be described by collection of continous connections a_A on patchs D_A that cover the whole base space. On the overlap of two patchs, D_A and D_B, the two gauge connections, a_A and a_B are gauge equivalent $a_B = a_A + \mathrm{d}f_{BA}$.
- Locally on each patch, the S^1-fiber boundle looks like $D_A \times S^1$, with cross section $|\psi_A(\xi^I)\rangle$, $\xi^I \in D_A$. On the overlap of two patchs, the two cross sections, $|\psi_A(\xi^I)\rangle$ and $|\psi_B(\xi^I)\rangle$, are related by $U(1)$ transformation $|\psi_B(\xi^I)\rangle = \mathrm{e}^{\mathrm{i} f_{BA}} |\psi_A(\xi^I)\rangle \to U(1)$**-bundle**.

The obstruction to have globally defined connection

Can we deform the gauge transformations $\mathrm{e}^{\mathrm{i}\, f_{BA}(\xi^I)}$ on the overlaps to 1, and turn a patchwise defined connection to a globally defined one?



- Consider a $U(1)$-bundle on S^2. We divide S^2 into two patchs with trivial topology (*ie* two disks). The overlap is the equator S^1. The transformation $U(\varphi) = \mathrm{e}^{\mathrm{i}\, f_{BA}(\varphi)}$ on the S^1 connects the connections on the two patchs

$$a_S = \underbrace{a_N - \mathrm{i}\, U^{-1} \mathrm{d} U}_{\text{correct form}} = \underbrace{a_N + \mathrm{d} f_{SN}}_{\text{incorrect form}}$$

- The non-trivial winding number of the transformation $U : S^1 \to U(1)$, due to $\pi_1(U(1)) = \mathbb{Z}$, is the obstruction to have globally defined connection $\to$ non-trivial $U(1)$-bundle on S^2 with

  Chern number $=$ winding number.

- On S^3 there is no non-trivial $U(1)$-bundle, but on $S^2 \times S^1$ or $S^1 \times S^1 \times S^2$ there is non-trivial $U(1)$-bundle.

- On S^4 there is non-trivial $SU(2)$-bundle, since $\pi_3(SU(2) = S^3) = \mathbb{Z}$.

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

Geometric phase is a quantum effect that can affect equation of motion

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 classical theroy (such as equation of motion and Lagrangian) that describes the motion of the above low energy neutron?*
- *What is the quantum Hamiltonian $\hat{H}$ that describes the quantum motion of the above low energy neutron?*

Our first guess:

- **Classical**: $m\ddot{\boldsymbol{x}} = -\partial V(\boldsymbol{x})$ and $L = \boldsymbol{p} \cdot \dot{\boldsymbol{x}} - \frac{1}{2}m\boldsymbol{p}^2 - \partial V(\boldsymbol{x})$, where $V(\boldsymbol{x}) = -|\mu_n \boldsymbol{B}(\boldsymbol{x})|$ is the effective potential energy.
  Quantum: $\hat{H} = -\frac{1}{2m_n}\partial^2 + V(\boldsymbol{x})$ *Is this guess correct?*

Schrödinger equation and coordinate basis

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

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

- 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 change 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 $\hat{H} = -\frac{1}{2m_n}\boldsymbol{\partial}^2 - |\mu_n\boldsymbol{B}(\boldsymbol{x})|$ is valid only when 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 $\mathrm{e}^{\mathrm{i}\phi(\boldsymbol{x})}\psi_{\text{tw}} = \psi(\boldsymbol{x})$

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

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

$$\hat{H}_{\text{tw}} = \hat{H}(\boldsymbol{\partial}+\mathrm{i}\boldsymbol{a},\boldsymbol{x}) = -\frac{1}{2m_n}(\boldsymbol{\partial}+\mathrm{i}\boldsymbol{a})^2 + V.$$

The above is derived for $\boldsymbol{a} = \boldsymbol{\partial}\phi$. But we assume it remains valid for general $\boldsymbol{a}$ → How geometric phase affects Schrödinger equation

Effective Hamiltonian for neutron in spin magnetic field

$$\hat{H}_{\text{eff}} = -\frac{1}{2m_n}(\partial + \mathrm{i}\boldsymbol{a})^2 + V$$

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.

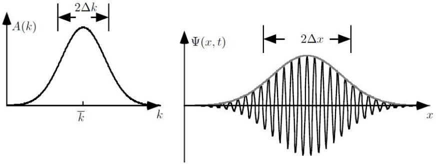
- $V(\boldsymbol{x})$ generates a potential force $\boldsymbol{F} = -\partial V$ on the particle.

- 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"* $\boldsymbol{b} = \partial \times \boldsymbol{a}$.

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 ($\hat{H} = -\frac{1}{2m}\partial^2 - \mu_n \boldsymbol{B}\cdot\boldsymbol{\sigma}$)

$$\begin{aligned}
\mathcal{L} &= \langle\psi_{\boldsymbol{x}_0(t),\boldsymbol{k}_0(t)}|\,\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}|\psi_{\boldsymbol{x}_0(t),\boldsymbol{k}_0(t)}\rangle - \langle\psi_{\boldsymbol{x}_0(t),\boldsymbol{k}_0(t)}|\hat{H}|\psi_{\boldsymbol{x}_0(t),\boldsymbol{k}_0(t)}\rangle \\
&= -\underbrace{\boldsymbol{a}'}_{=0}\cdot\dot{\boldsymbol{x}}_0 - \underbrace{\boldsymbol{a}''}_{\boldsymbol{x}_0}\cdot\dot{\boldsymbol{k}}_0 - \underbrace{\boldsymbol{a}(\boldsymbol{x}_0)}_{-\,\mathrm{i}\,\langle\boldsymbol{n}|\partial_{\boldsymbol{x}_0}|\boldsymbol{n}\rangle}\cdot\dot{\boldsymbol{x}}_0 - \frac{\boldsymbol{k}_0^2}{2m_n} - |\mu_n\boldsymbol{B}(\boldsymbol{x}_0)| \\
&= -\boldsymbol{x}_0\cdot\dot{\boldsymbol{k}}_0 - \boldsymbol{a}(\boldsymbol{x}_0)\cdot\dot{\boldsymbol{x}}_0 - \frac{\boldsymbol{k}_0^2}{2m_n} + |\mu_n\boldsymbol{B}(\boldsymbol{x}_0)| \\
&\approx \boldsymbol{p}_0\cdot\dot{\boldsymbol{x}}_0 - \boldsymbol{a}(\boldsymbol{x}_0)\cdot\dot{\boldsymbol{x}}_0 - \frac{\boldsymbol{p}_0^2}{2m_n} - V(\boldsymbol{x}_0). \qquad (\hbar = 1 \text{ unit})
\end{aligned}$$

Obtain classical equation of motion

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

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

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

we obtain the phase space equation of motion

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

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

Geometric phase = orbital magnetic field

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

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

- 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 $\boldsymbol{a} = -\frac{e}{c}\boldsymbol{A}$ (or $\boldsymbol{a} = -\frac{e}{\hbar c}\boldsymbol{A}$ in $\hbar \neq 1$ unit, $[\boldsymbol{a}] = \text{Length}^{-1}$).

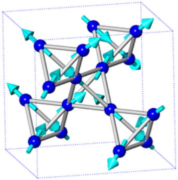
- **The geometric meaning of magnetic field**

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

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

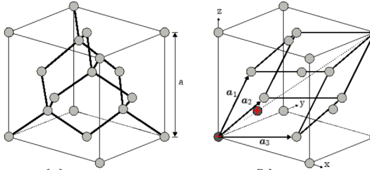
- If there is one flux quantum per $(10^{-8}m)^2$, then $B = 4.135667516 \times 10^{-15}/(10^{-8})^2 = 41\text{T}$ (About the highest static magnetic field produced)

- 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 $B_{\text{spin}} = 4.135667516 \times 10^{-15}/(10^{-9})^2 = 4100\text{T}$

Geometric phases in energy bands of a crystal

- Hopping Hamiltonian

Si



(a) (b)

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

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

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

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

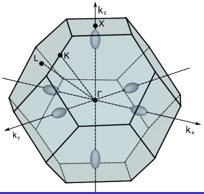
- The energy bands $\epsilon_{\boldsymbol{k}}$ are eigenvalues of $M_{\alpha\beta}(\boldsymbol{k})$

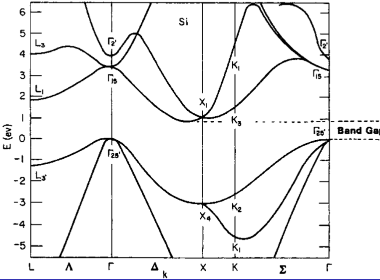
Si bands

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

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

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





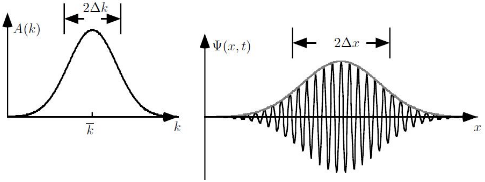
Dynamics of an electron in semiconductor

The standard theory

- Quantum dynamics: $H(\hat{\boldsymbol{p}}) = \epsilon(\hat{\boldsymbol{p}})$, $\hat{p} = -\mathrm{i}\boldsymbol{\partial} \to$
  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 $\mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{x}}\,\mathrm{e}^{-\mathrm{i}\,\frac{\epsilon(\boldsymbol{k})t}{\hbar}}\psi(\boldsymbol{k})\rangle$.

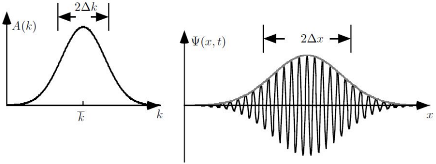
  With potential term, the Hamiltonian is changed to
  $H(\hat{\boldsymbol{p}}, \hat{\boldsymbol{x}}) = \epsilon(\hat{\boldsymbol{p}}) + V(\hat{\boldsymbol{x}})$, where $[\hat{p}^i, \hat{x}^j] = -\mathrm{i}\delta_{ij}$, or
  $H(\hat{\boldsymbol{p}}, \hat{\boldsymbol{x}}) = \epsilon(-\mathrm{i}\boldsymbol{\partial}) + V(\hat{\boldsymbol{x}})$
- Classical dynamics: $\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{O}\rangle = \mathrm{i}\langle[H, \hat{O}]\rangle \to$

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



- *The standard theory is wrong.*

- Consider wavepacket with space-time dependent spin



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

Phase space Lagrangian ($\hbar \neq 1$ unit)

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

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

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

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

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

$$\begin{aligned} L &= \boldsymbol{p} \cdot \dot{\boldsymbol{x}} + \frac{e}{c}\boldsymbol{A}(\boldsymbol{x}) \cdot \dot{\boldsymbol{x}} - \tilde{\boldsymbol{a}}(\boldsymbol{p}/\hbar) \cdot \dot{\boldsymbol{p}} - \frac{\boldsymbol{p}^2}{2m_n} - V(\boldsymbol{x}) \\ &= \hbar[\boldsymbol{k} \cdot \dot{\boldsymbol{x}} - \boldsymbol{a}(\boldsymbol{x}) \cdot \dot{\boldsymbol{x}} - \tilde{\boldsymbol{a}}(\boldsymbol{k}) \cdot \dot{\boldsymbol{k}}] - \frac{\boldsymbol{p}^2}{2m_n} - V(\boldsymbol{x}) \end{aligned}$$

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.

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 $H = \frac{\hbar^2 \boldsymbol{k}^2}{2m} + V(\boldsymbol{x})$, we obtain

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

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 $\boldsymbol{x} = \boldsymbol{x}_\omega \mathrm{e}^{-\mathrm{i}\omega t}$:

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

Effect of D_{ij} disappear for DC conductance, for the first way to model dissipation $F_{\text{friction}} = -\gamma\dot{x}^i$.

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} also disappear for DC conductance, for the second way to model dissipation $F_{\text{friction}} = -\gamma \partial_{p_i} H$. But the result is different from the first way $F_{\text{friction}} = -\gamma \dot{x}^i$.

Hydrodynamics in phase space:
In the third way to model dissipation, we find that D_{ij} has effect on DC conductance!

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

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

where the phase space curvature ($I = x^1, x^2, x^3, k^1, k^2, k^3$) is given by

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

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

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

Density distribution in phase space

- To set up phase space hydrodynamics, we first 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 ($\mathcal{J}^I = g\dot{\xi}^I$):

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

  See Appendix at the end of this note for derivation.

- When $\mathrm{Pf}[b(\xi^I)] = 1$, say when either $b_{ij} = 0$ or $\tilde{b}_{ij} = 0$, the conservation of particle number reduces to $\frac{\partial g}{\partial t} + \partial_I \mathcal{J}^I = 0$.

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

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

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

- $(\boldsymbol{x},\boldsymbol{k})$-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

Impurity scattering $\to$ dissipation.

- We model large Δk redistribution caused by impurities 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.

- **Local chemical potential $\mu(\boldsymbol{x})$ and local temperature $T(\boldsymbol{x})$**:

- $\delta g = (g - g_0)/\tau$ 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 local 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.

- Impurity scattering conserve the energy density in $\boldsymbol{x}$-space $n_E(\boldsymbol{x}) = \int \mathrm{Pf}(b, \tilde{b}) \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}\ E(\boldsymbol{x}, \boldsymbol{k}) g$. The local temperature $T(\boldsymbol{x})$ satisfies

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

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**

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

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

\- Make another assumption $\frac{\partial_{x_i} \delta g}{\delta g} \ll \frac{1}{\tau v^i} = \frac{1}{l}$. Since $\hbar \dot{k}_i = eE_i - \hbar b_{ij} v^j$:

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

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

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

Note that (try to show this in 1-dimension)

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

where $\partial G_0(\epsilon)/\partial \epsilon = g_0(\epsilon)$. Keeping only linear E_i term

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

- **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

Thouless

For a filled band, $g_0 = 1$

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

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

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

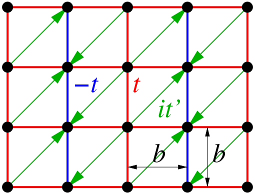
$$\mathrm{i}\, \tilde{a}_i = \langle \psi(\boldsymbol{k}) | \partial_{k_i} | \psi(\boldsymbol{k}) \rangle.$$

We 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?

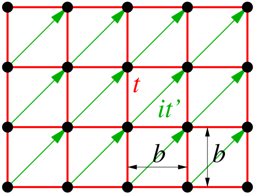
Complex hopping to break time-reversal and parity symm.



- Conductance $j_y = \sigma_{xy} E_x$, $j_x = E_y = 0$.

  Under time reversal $t \to -t$:
  $\boldsymbol{E} \to \boldsymbol{E}, \quad \boldsymbol{j} \to -\boldsymbol{j}, \quad \sigma_{xy} \to -\sigma_{xy}$

  Under parity $(x, y) \to (x, -y)$:
  $(E_x, E_y) \to (E_x, -E_y), \quad (j_x, j_y) \to (j_x, -j_y), \quad \sigma_{xy} \to -\sigma_{xy}$

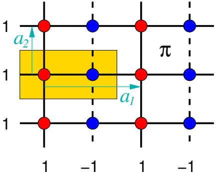


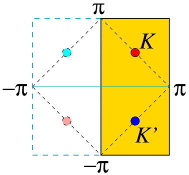
- Use complex hopping to generate **uniform flux** and break time-reversal and parity symmetries.
  $\to$ **Chern insulator**

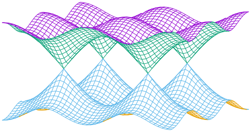
  Staggered flux breaks time-reversal symmetry but not parity symmetry.
  $\to$ not Chern insulator

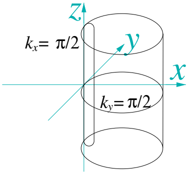
- Next we compute the hopping matrix in $\boldsymbol{k}$-space

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









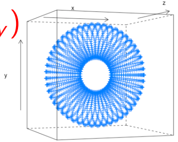
Hopping matrix in $\boldsymbol{k}$-space ($\boldsymbol{a}_1 = 2\boldsymbol{x}$, $\boldsymbol{a}_2 = \boldsymbol{y}$): plot $\boldsymbol{n}(k_x, k_y)$

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

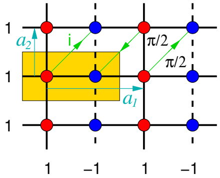
- $M(k) = \boldsymbol{v}(\boldsymbol{k})\cdot\boldsymbol{\sigma}$: $\epsilon = \pm|\boldsymbol{v}(\boldsymbol{k})|$. The vector field $\boldsymbol{v}(\boldsymbol{k})$ on B.Z.:

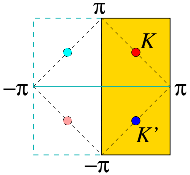
$$v_x = -t - t\cos(2k_x), \quad v_y = -t\sin(2k_x), \quad v_z = -2t\cos(k_y).$$
$$|\boldsymbol{v}| = t\sqrt{2 + 2\cos(2k_x) + 4\cos^2(k_y)} = t\sqrt{4\cos^2(k_x) + 4\cos^2(k_y)}.$$

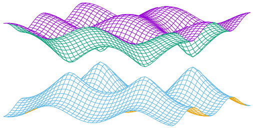
- Eigenstate in conduction band $|\boldsymbol{n}(\boldsymbol{k})\rangle$, plot $\boldsymbol{n}(k_x, k_y)$
$\boldsymbol{n}(\boldsymbol{k}) = \boldsymbol{v}(\boldsymbol{k})/|\boldsymbol{v}(\boldsymbol{k})|$, has geometric connection
$\mathrm{i}\,\tilde{a}_i(\boldsymbol{k}) = \langle\boldsymbol{n}(\boldsymbol{k})|\partial_{k_i}|\boldsymbol{n}(\boldsymbol{k})\rangle$: $\tilde{b}_{xy} = \partial_{k_x}\tilde{a}_y - \partial_{k_y}\tilde{a}_x \neq 0$
$\oint_K \mathrm{d}\boldsymbol{k}\cdot\tilde{\boldsymbol{a}} = \pi$, $\oint_{K'} \mathrm{d}\boldsymbol{k}\cdot\tilde{\boldsymbol{a}} = \pi$ $\to$ two π-flux tubes.

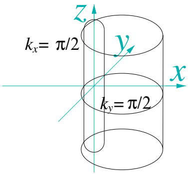


$\pi/2$-flux state: complex hopping $\to$ Chern insulator









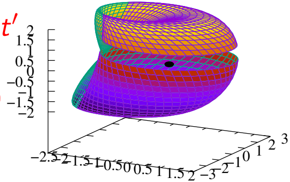
Hopping matrix in $\boldsymbol{k}$-space ($\boldsymbol{a}_1 = 2\boldsymbol{x}$, $\boldsymbol{a}_2 = \boldsymbol{y}$): $M(\boldsymbol{k}) =$

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

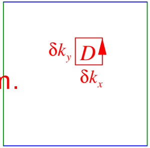
- $M(k) = \boldsymbol{v}(\boldsymbol{k})\cdot\boldsymbol{\sigma}$: $\epsilon = \pm|\boldsymbol{v}(\boldsymbol{k})|$. The vector field $\boldsymbol{v}(\boldsymbol{k})$ on B.Z.:

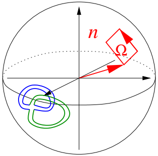
  $v_x = -t - t\cos(2k_x) - t'\sin(k_y) + t'\sin(k_y + 2k_x)$,
  $v_y = -t\sin(2k_x) - t'\cos(k_y) - t'\cos(k_y + 2k_x)$, $v_z = -2t\cos(k_y)$.

- Eigenstate in conduction band $|\boldsymbol{n}(\boldsymbol{k})\rangle$, $t = t'$
  $\boldsymbol{n}(\boldsymbol{k}) = \boldsymbol{v}(\boldsymbol{k})/|\boldsymbol{v}(\boldsymbol{k})|$, 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) $= 1$
  Chern insulator (IQH state)



How to compute the Chern number





- 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:

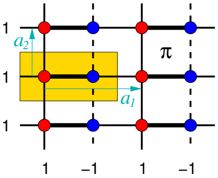
$$\tilde{B}\delta k_x \delta k_y = \frac{1}{2}\boldsymbol{n} \cdot \Big([\boldsymbol{n}(\boldsymbol{k} + \delta k_x \boldsymbol{x}) - \boldsymbol{n}(\boldsymbol{k})] \times [\boldsymbol{n}(\boldsymbol{k} + \delta k_y \boldsymbol{y}) - \boldsymbol{n}(\boldsymbol{k})] \Big)$$

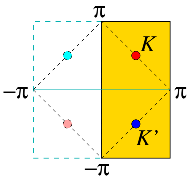
$$\tilde{B}(\boldsymbol{k}) = \frac{1}{2}\boldsymbol{n} \cdot [\partial_{k_x}\boldsymbol{n}(\boldsymbol{k}) \times \partial_{k_y}\boldsymbol{n}(\boldsymbol{k})]$$

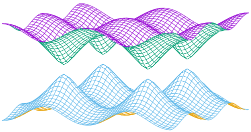
- Compute Chern number (the wrapping number):

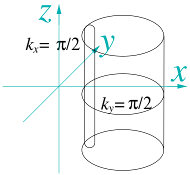
$$(4\pi)^{-1} \int_{B.Z.} \mathrm{d}^2 k \ \boldsymbol{n} \cdot [\partial_{k_x}\boldsymbol{n}(\boldsymbol{k}) \times \partial_{k_y}\boldsymbol{n}(\boldsymbol{k})] = \text{Chern number}$$

Dimmer state









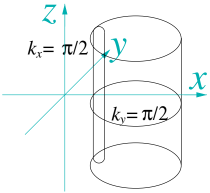
Hopping matrix in $\boldsymbol{k}$-space ($\boldsymbol{a}_1 = 2\boldsymbol{x}$, $\boldsymbol{a}_2 = \boldsymbol{y}$): plot $\boldsymbol{n}(k_x, k_y)$

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

- $M(k) = \boldsymbol{v}(\boldsymbol{k}) \cdot \boldsymbol{\sigma}$: $\epsilon = \pm|\boldsymbol{v}(\boldsymbol{k})|$. The vector field $\boldsymbol{v}(\boldsymbol{k})$ on B.Z.:

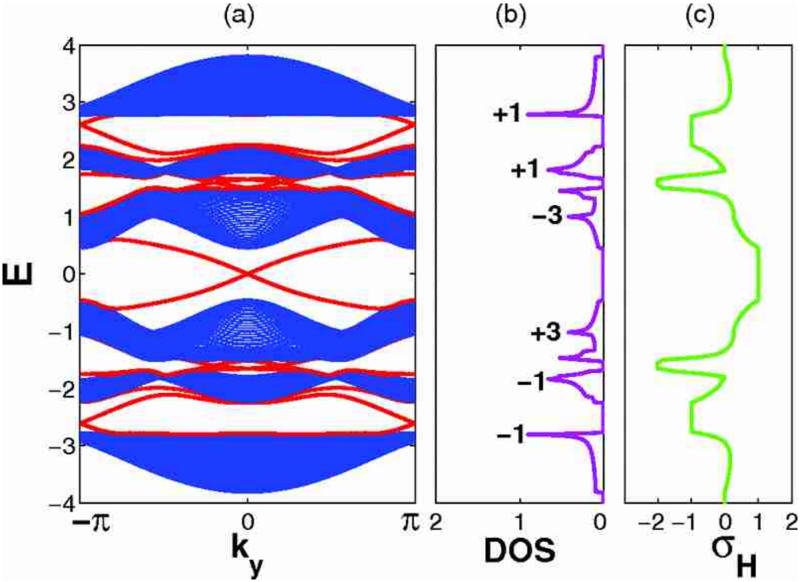
  $v_x = -t' - t\cos(2k_x)$, $v_y = -t\sin(2k_x)$, $v_z = -2t\cos(k_y)$.

- Eigenstate in conduction band $|\boldsymbol{n}(\boldsymbol{k})\rangle$,
  $\boldsymbol{n}(\boldsymbol{k}) = \boldsymbol{v}(\boldsymbol{k})/|\boldsymbol{v}(\boldsymbol{k})|$, has geometric connection
  $\mathrm{i}\,\tilde{a}_i(\boldsymbol{k}) = \langle \boldsymbol{n}(\boldsymbol{k})|\partial_{k_i}|\boldsymbol{n}(\boldsymbol{k})\rangle$: $\tilde{b}_{xy} = \partial_{k_x}\tilde{a}_y - \partial_{k_y}\tilde{a}_x \neq 0$
  $\to$ The wrapping number (Chern number) $= 0$



Atomic insulator

Chern number of the bands



Appendix: Hydrodynamic equation and continuity equation (for $b_{IJ} = const.$)

- **Hydrodynamic equation**

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

- **Continuity equation** conservation of particle number ($b_{IJ} = const.$):

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

They are equivalent:

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

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

Appendix: continuity equation (for $b_{IJ} \neq const.$)

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

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

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

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

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

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

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

- The form of the hydrodynamic EOM remain unchanged:

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

Appendix: continuity equation (for $b_{IJ} \neq const.$)

- The form of the continuity 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 $M_{IJ} = \frac{\partial \tilde{\xi}^I}{\partial \xi^J}$)

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

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

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

Appendix: continuity equation = Hydrodynamic equation

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

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

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 $\frac{\partial g}{\partial t} - b^{IJ}\partial_I g\partial_J H = 0$.

Appendix: 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.

Appendix: 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:

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

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

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

Diffusion current

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

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

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

Appendix: Hydrodynamics in phase space with diffusion

For classical particles (high temperature limit $g \ll 1$)

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

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?