

### Central charge in condensed matter systems: (one example)

In condensed matter physics, 1D Fermi gas and Bose gas has the same Central charge  $C=1$ . They are totally equivalent to each other. In 1D, one can turn bosons into fermions or fermions into bosons and vice versa, which is known as “bosonization”.

For  $C < 1$ , we know pretty much everything about the critical behavior (scaling laws) by knowing the value of  $C$ .

For  $C \geq 1$ , a little bit more complicated. Some additional symmetry could be helpful (affine Lie algebras)

## 3.4. Example II: Phase of Bloch waves

### 3.4.1. Phase of a Bloch wavefunction

A particle moving in a periodic potential:

$$\left[ -\frac{1}{2m} \nabla^2 + V(\vec{r}) \right] \psi(\vec{r}) = \epsilon \psi(\vec{r}) \quad (3.55)$$

with

$$V(\vec{r}) = V(\vec{r} + \vec{a}_i) \quad (3.56)$$

Eigen-wavefunctions: Bloch waves

$$\psi_{n,k}(r) = u_{n,k}(r) \exp(i k r) \quad (3.57)$$

■ Q: Phase of  $u_{n,k}(r)$ ?

■ A: Doesn't matter. Phase itself is unimportant.

Bloch waves are invariant under a global phase shift in the momentum space. (Same as other quantum states)

If  $\psi_{n,k}(r) = u_{n,k}(r) \exp(i k r)$  is a Bloch wave, then  $\psi'_{n,k}(r) = e^{i \phi} u_{n,k}(r) \exp(i k r)$  is the same eigen state

In addition, Bloch waves are invariant under a local phase shift in the momentum space. (new and important)

If  $\psi_{n,k}(r) = u_{n,k}(r) \exp(i k r)$  is a Bloch wave, then  $\psi'_{n,k}(r) = e^{i \phi(k)} u_{n,k}(r) \exp(i k r)$  is the same eigen state

$$\left[ -\frac{1}{2m} \nabla^2 + V(\vec{r}) \right] \psi_{n,k}(r) = \epsilon \psi_{n,k}(r) \quad (3.58)$$

$$\left[ -\frac{1}{2m} \nabla^2 + V(\vec{r}) \right] \psi'_{n,k}(r) = \left[ -\frac{1}{2m} \nabla^2 + V(\vec{r}) \right] e^{i \phi(k)} \psi_{n,k}(r) = \quad (3.59)$$

$$e^{i \phi(k)} \left[ -\frac{1}{2m} \nabla^2 + V(\vec{r}) \right] \psi_{n,k}(r) = e^{i \phi(k)} \epsilon \psi_{n,k}(r) = \epsilon e^{i \phi(k)} \psi_{n,k}(r) = \epsilon \psi'_{n,k}(r)$$

The system is invariant under a local phase shift in the momentum space.

Requirement to have such a local symmetry.

1 Momentum conservation (no impurities)

2. electron interactions

So, a particle with momentum  $k$  always has momentum  $k$ . Bloch waves with different momentum doesn't talk to each other. So their phase can change independently.

## 3.5. Local phase symmetry

### 3.5.1. How to describe this local phase degrees of freedom?

Q: Do we know something similar?

A: Yes, we know a similar local phase degrees of freedom. Not in the  $k$ -space, but in the real space, which is the gauge symmetry.

This section, I review some basic knowledge we learned in the quantum mechanics class.

Reference: Landau and Lifshitz, Quantum Mechanics (non-relativistic theory).

### 3.5.2. Global $U(1)$ phase symmetry in real space and particle conservation

Schrodinger equation is invariant under global phase shift in the real space.

$$i \frac{\partial}{\partial t} \psi(r, t) = -\frac{\nabla^2}{2m} \psi(r, t) + V(r) \psi(r, t) \quad (3.60)$$

Define:  $\psi'(r) = e^{i\phi} \psi(r)$  where  $\phi$  is a constant (We shift the phase of every point by the same amount, which is known as a global phase change)

$$\begin{aligned} i \frac{\partial}{\partial t} \psi'(r, t) &= i \frac{\partial}{\partial t} [e^{i\phi} \psi(r, t)] = \\ e^{i\phi} \left[ i \frac{\partial}{\partial t} \psi(r, t) \right] &= e^{i\phi} \left[ -\frac{\nabla^2}{2m} \psi(r, t) + V(r) \psi(r, t) \right] = -\frac{\nabla^2}{2m} e^{i\phi} \psi(r, t) + V(r) e^{i\phi} \psi(r, t) = -\frac{\nabla^2}{2m} \psi'(r, t) + V(r) \psi'(r, t) \end{aligned} \quad (3.61)$$

■ Key:  $\phi$  is a constant, so that  $\frac{\partial}{\partial t} e^{i\phi} = e^{i\phi} \frac{\partial}{\partial t}$  and  $\nabla e^{i\phi} = e^{i\phi} \nabla$

$\psi'(r)$  follows the same equation as  $\psi(r)$ . The system is invariance under a global phase shift, which is known as a global  $U(1)$  phase symmetry.

Symmetry implies conservation law. Here, this symmetry means particle conservation (total probability density of a wavefunction is conserved  $\partial_t \int d r \langle \psi | \psi \rangle = 0$ ).

Demonstration (no a proof)

Translational symmetry  $x \rightarrow x + a$  implies the conservation of  $-i \partial_x$ . So here, for  $U(1)$  phase symmetry, we expect the conservation of  $-i \partial_\phi$ . Here I show that  $\int d r \langle \psi | -i \partial_\phi | \psi \rangle = \int d r \langle \psi | \psi \rangle$ . So the conservation of  $-i \partial_\phi$  implies the conservation of total probability density.

For a wavefunction  $\psi(r, t)$

$$-i \partial_\phi \psi(r, t) = -i \frac{\psi(r, t) e^{i\delta\phi} - \psi(r, t)}{\delta\phi} = -i \frac{e^{i\delta\phi} - 1}{\delta\phi} \psi(r, t) = -i \frac{(1 + i\delta\phi) - 1}{\delta\phi} \psi(r, t) = \psi(r, t) \quad (3.62)$$

$$\langle \psi | -i \partial_\phi | \psi \rangle = \int d r \psi^*(r, t) [-i \partial_\phi \psi(r, t)] = \int d r \psi^*(r, t) \psi(r, t) = \int d r (|\psi(r, t)|^2) \quad (3.63)$$

So  $\int d r (|\psi(r, t)|^2)$  is conserved.

Here, the phase change  $\phi$  is a constant, instead of an arbitrary function. What will happen if  $\phi$  is a function of  $r$ ?

### 3.5.3. Local $U(1)$ phase symmetry in real space and gauge fields

Define: a local phase shift  $\psi'(r, t) = e^{i\phi(r, t)} \psi(r, t)$

Q: Is Schrodinger equation invariant under local phase shift?

A: No.

Key:  $\phi$  is a function of  $t$  and  $r$ , so that  $\frac{\partial}{\partial t} e^{i\phi} \neq e^{i\phi} \frac{\partial}{\partial t}$  and  $\nabla e^{i\phi} \neq e^{i\phi} \nabla$

$$\begin{aligned} i \frac{\partial}{\partial t} \psi'(r, t) &= i \frac{\partial}{\partial t} [e^{i\phi(r, t)} \psi(r, t)] = \\ &= \frac{\partial \phi(r, t)}{\partial t} e^{i\phi(r, t)} \psi(r, t) + i e^{i\phi(r, t)} \frac{\partial}{\partial t} \psi(r, t) = \frac{\partial \phi(r, t)}{\partial t} e^{i\phi(r, t)} \psi(r, t) - \frac{\partial \phi(r, t)}{\partial t} e^{i\phi(r, t)} \psi(r, t) - \frac{\nabla^2}{2m} e^{i\phi(r, t)} \psi(r, t) + e^{i\phi(r, t)} V(r) \psi(r, t) \\ &= -\frac{\partial \phi(r, t)}{\partial t} \psi'(r, t) - e^{i\phi(r, t)} \frac{\nabla^2}{2m} [e^{-i\phi(r, t)} \psi'(r, t)] + V(r) \psi'(r, t) = \\ &= -\frac{\partial \phi(r, t)}{\partial t} \psi'(r, t) - \frac{\nabla^2}{2m} \psi'(r, t) + V(r) \psi'(r, t) + \frac{i}{m} [\nabla \phi(r, t) \cdot \nabla \psi'(r, t)] + \frac{1}{2m} [i \nabla^2 \phi(r, t) \psi'(r, t) + (\nabla \phi(r, t))^2 \psi'(r, t)] \end{aligned} \quad (3.64)$$

$$= -\frac{\partial \phi(r, t)}{\partial t} \psi'(r, t) - \frac{\nabla^2}{2m} \psi'(r, t) + V(r) \psi'(r, t) + \frac{i}{m} [\nabla \phi(r, t) \cdot \nabla \psi'(r, t)] + \frac{1}{2m} [i \nabla^2 \phi(r, t) \psi'(r, t) + (\nabla \phi(r, t))^2 \psi'(r, t)]$$

$$\left( i \frac{\partial}{\partial t} + \frac{\partial \phi(r, t)}{\partial t} \right) \psi'(r, t) = \frac{[-i \nabla - \nabla \phi(r, t)]^2}{2m} \psi'(r, t) + V(r) \psi'(r, t) \quad (3.65)$$

$$\frac{[-i \nabla - \nabla \phi(r, t)]^2}{2m} \psi'(r, t) = \frac{[-i \nabla - \nabla \phi(r, t)] \cdot [-i \nabla - \nabla \phi(r, t)]}{2m} \psi'(r, t) = \frac{[-i \nabla - \nabla \phi(r, t)]}{2m} \cdot [-i \nabla \psi'(r, t) - \psi'(r, t) \nabla \phi(r, t)] =$$

$$-\frac{\nabla^2 \psi'(r, t)}{2m} + \frac{i}{2m} \cdot [\psi'(r, t) \nabla \phi(r, t)] - \frac{\nabla \phi(r, t)}{2m} \cdot [-i \nabla \psi'(r, t) - \psi'(r, t) \nabla \phi(r, t)]$$

$$= -\frac{\nabla^2 \psi'(r, t)}{2m} + \frac{i}{m} [\nabla \psi'(r, t) \cdot \nabla \phi(r, t)] + \frac{i}{2m} [\psi'(r, t) \nabla^2 \phi(r, t)] + \frac{[\nabla \phi(r, t)]^2}{2m} \psi'(r, t) \quad (3.66)$$

Q: Can we make the Schrodinger equation invariant under local phase shift?

A: Yes. Using charge particles.

Schrodinger equation for a particle with charge  $e$ . Just change the momentum operator  $\vec{p}$  into  $\vec{p} + e \vec{A} / c$ , where  $\vec{A}$  is the vector potential, and change  $i \partial_t$  into  $i \partial_t - e \Phi$ , where  $\Phi$  is the Electric potential. (minimal coupling).

$$(i \hbar \partial_t - e \Phi) \psi(r, t) = \left[ \frac{1}{2m} \left( -i \hbar \nabla - \frac{e}{c} \vec{A} \right)^2 \right] \psi(r, t) + V(r) \psi(r, t) \quad (3.67)$$

$$\left( i \hbar \partial_t - e \Phi + \hbar \frac{\partial \phi(r, t)}{\partial t} \right) \psi'(r, t) = \frac{1}{2m} \left( -i \hbar \nabla - \frac{e}{c} \vec{A} - \hbar \nabla \phi(r, t) \right)^2 \psi'(r, t) + V(r) \psi'(r, t) \quad (3.68)$$

If we define:

$$\Phi' = \Phi - \frac{\hbar}{e} \frac{\partial \phi(r, t)}{\partial t} \quad (3.69)$$

and

$$\vec{A}' = \vec{A} + \frac{c \hbar}{e} \nabla \phi(r, t) \quad (3.70)$$

we got:

$$(i \hbar \partial_t - e \Phi') \psi'(r, t) = \frac{1}{2m} \left( -i \hbar \nabla - \frac{e}{c} \vec{A}' \right)^2 \psi'(r, t) + V(r) \psi'(r, t) \quad (3.71)$$

The SE is invariant under a local phase shift, if we changes the potential and vector potential as defined above. The change of  $\Phi$  and  $A$  is just a gauge transformation. It doesn't change any physics (Same E and B). So we say that the SE for a charged particle is invariant under local phase shift.

Because this local gauge shift is related with a gauge transformation, sometime we just call this local phase shift a gauge transformation.

In another convention, which is probably more widely used, on absorb the constant  $c \hbar/e$  into the definition of  $\phi$ , so the SE is invariant under gauge transformation:

$$\Phi \rightarrow \Phi' = \Phi - \frac{\partial \phi(r, t)}{c \partial t} \quad (3.72)$$

$$\vec{A} \rightarrow \vec{A}' = \vec{A} + \nabla \phi(r, t) \quad (3.73)$$

$$\Psi(r, t) \rightarrow \Psi'(r, t) = \Psi(r, t) \exp \left( i \frac{e}{c \hbar} \phi \right) \quad (3.74)$$

Bottom line: local phase symmetry is directly related with a gauge field. For the Bloch waves, which as a local phase symmetry in the k-space, we should also think about "gauge fields" but in k-space.

### 3.6. Berry connection and Berry curvature: “Vector potential” and “magnetic fields” in k-space

#### 3.6.1. Berry connection

Define the Berry connection:

$$\vec{\mathcal{A}}_n = -i \left\langle u_{n,k} \left| \nabla_k \right| u_{n,k} \right\rangle \quad (3.75)$$

In some literature, there is no minus sign in the definition. In some references,  $k$  is the momentum and in some others  $k$  is the wave vector (they are different by a factor of  $\hbar$ ). Here, I choose  $k$  to be the wave vector.

This is a gauge like field in the  $k$ -space, pretty similar to the vector potential  $\vec{A}$ .

Under a local phase shift:

$$|u_{n,k}\rangle \rightarrow e^{i\phi_n(k)} |u_{n,k}\rangle \quad (3.76)$$

$$\vec{\mathcal{A}}_n \rightarrow \vec{\mathcal{A}}_n' = -i \left\langle u_{n,k} \left| e^{-i\phi_n(k)} \nabla_k e^{i\phi_n(k)} \right| u_{n,k} \right\rangle = -i \left\langle u_{n,k} \left| \nabla_k \right| u_{n,k} \right\rangle + \nabla_k \phi_n(k) \langle u_{n,k} | u_{n,k} \rangle = \vec{\mathcal{A}}_n + \nabla_k \phi_n(k) \quad (3.77)$$

$\vec{\mathcal{A}}_n$  changes like a gauge field (the vector potential). But  $\vec{\mathcal{A}}_n$  lives in the  $k$  – space and all derivatives are derivatives of  $k$ , instead of  $r$ .

#### 3.6.2. Berry curvature

We know that the vector potential is not a physical observable, and its value depends on the gauge choice. The quantity with physical meaning is the curl of it, which is the magnetic field  $B$ . Here, it is the same story.

$$\mathcal{F}_n = \nabla_k \times \vec{\mathcal{A}}_n = -i \epsilon_{ij} \partial_{k_i} \langle u_{n,k} | \partial_{k_j} | u_{n,k} \rangle = -i \epsilon_{ij} \langle \partial_{k_i} u_{n,k} | \partial_{k_j} u_{n,k} \rangle \quad (3.78)$$

#### 3.6.3. The position operator in a lattice

**We know that without lattice,  $p = -i\hbar \nabla_r$  and  $r = i\hbar \nabla_p$ . What will happen if we have a lattice?**

In the continuum we know that  $p = -i\hbar \nabla_r$  and  $r = i\hbar \nabla_p$ . To see this, we simply use the plan wave expansions and write any wave-functions in a superposition of plan waves.

$$\Psi(\vec{k}) = \int d\vec{r} \Psi(\vec{r}) e^{-i\vec{k} \cdot \vec{r}} \quad (3.79)$$

$$\Psi(\vec{r}) = \int d\vec{k} \Psi(\vec{k}) e^{i\vec{k} \cdot \vec{r}} \quad (3.80)$$

To prove  $r = i\hbar \nabla_p$ , the most straight-forward way is to use

$$\Psi(\vec{k}) = \int d\vec{r} \Psi(\vec{r}) e^{-i\vec{k} \cdot \vec{r}} \quad (3.81)$$

$$\vec{r} \Psi(\vec{k}) = \int d\vec{r} \vec{r} \Psi(\vec{r}) e^{-i\vec{k} \cdot \vec{r}} = \int d\vec{r} \Psi(\vec{r}) \left[ i \partial_k e^{-i\vec{k} \cdot \vec{r}} \right] = i \partial_k \int d\vec{r} \Psi(\vec{r}) e^{-i\vec{k} \cdot \vec{r}} = i \partial_k \Psi(\vec{k}) \quad (3.82)$$

Here, we will show a different (less straightforward approach), which can be generalized to Bloch waves easily using the inverse transformation:

$$\Psi(\vec{r}) = \int d\vec{k} \Psi(\vec{k}) e^{i\vec{k} \cdot \vec{r}} \quad (3.83)$$

Here we ask the question, what operator  $\vec{X}$  can we use to make the two sides of the equation equal. Because we have an position operator on the l.h.s., this means that  $\vec{X}$  is the position operator.

$$\vec{r} \Psi(\vec{r}) = \int d\vec{k} \vec{X} \Psi(\vec{k}) e^{i\vec{k} \cdot \vec{r}} \quad (3.84)$$

$$\vec{r} \Psi(\vec{r}) = \int d\vec{k} \vec{r} \Psi(\vec{k}) e^{i\vec{k}\cdot\vec{r}} = \int d\vec{k} \Psi(\vec{k}) [-i \vec{\partial}_k e^{i\vec{k}\cdot\vec{r}}] = \int d\vec{k} [i \vec{\partial}_k \Psi(\vec{k})] e^{i\vec{k}\cdot\vec{r}} \quad (3.85)$$

So we have  $\vec{X} = i \vec{\nabla}_k$

For Bloch waves, we can do the same thing. In general, any wavefunction can be written as a superposition of the Bloch waves:

$$\Psi(\vec{r}) = \sum_n \int d\vec{k} \Psi_n(\vec{k}) \psi_{n,k}(\vec{r}) = \sum_n \int d\vec{k} \Psi_n(\vec{k}) u_{n,k}(\vec{r}) e^{i\vec{k}\cdot\vec{r}} \quad (3.86)$$

This is similar to a Fourier transform, but we use Bloch waves as basis instead of the planes. Here the inverse transformation is not so straightforward to write down.

If I want to know the position of this wavefunction:  $\Psi(r)$ , we simply use  $\vec{r} \Psi(\vec{r})$ , and now we ask what operator  $\vec{X}$  can we use to satisfies:

$$\vec{r} \Psi(\vec{r}) = \sum_n \int d\vec{k} \vec{X} \Psi_n(\vec{k}) \psi_{n,k}(\vec{r}) \quad (3.87)$$

This  $\vec{X}$  operator is the position operator in k-space

$$\begin{aligned} \vec{r} \Psi(\vec{r}) &= \vec{r} \sum_n \int d\vec{k} \Psi_n(\vec{k}) \psi_{n,k}(\vec{r}) = \sum_n \int d\vec{k} \Psi_n(\vec{k}) u_{n,k}(\vec{r}) \vec{r} e^{i\vec{k}\cdot\vec{r}} = \sum_n \int d\vec{k} \Psi_n(\vec{k}) u_{n,k}(\vec{r}) (-i \vec{\partial}_k e^{i\vec{k}\cdot\vec{r}}) = \\ &= \sum_n \int d\vec{k} [i \vec{\partial}_k \Psi_n(\vec{k})] u_{n,k}(\vec{r}) e^{i\vec{k}\cdot\vec{r}} = \sum_n \int d\vec{k} [i \vec{\partial}_k \Psi_n(\vec{k}) u_{n,k}(\vec{r}) + \Psi_n(\vec{k}) i \vec{\partial}_k u_{n,k}(\vec{r})] e^{i\vec{k}\cdot\vec{r}} \end{aligned} \quad (3.88)$$

$$\begin{aligned} \vec{r} \Psi(\vec{r}) &= \sum_n \int d\vec{k} [i \vec{\partial}_k \Psi_n(\vec{k})] \psi_{n,k}(\vec{r}) + \Psi_n(\vec{k}) \int d\vec{r}' \delta(\vec{r} - \vec{r}') i \vec{\partial}_k u_{n,k}(\vec{r}') e^{i\vec{k}\cdot\vec{r}} \\ &= \sum_n \int d\vec{k} [i \vec{\partial}_k \Psi_n(\vec{k})] \psi_{n,k}(\vec{r}) + \Psi_n(\vec{k}) \int d\vec{r}' \sum_m u_{m,k}^*(\vec{r}') u_{m,k}(\vec{r}) i \vec{\partial}_k u_{n,k}(\vec{r}') e^{i\vec{k}\cdot\vec{r}} \\ &= \sum_n \int d\vec{k} \{ i \vec{\partial}_k \Psi_n(\vec{k}) \psi_{n,k}(\vec{r}) + \Psi_n(\vec{k}) \sum_m u_{m,k}(\vec{r}) [\int d\vec{r}' u_{m,k}^*(\vec{r}') i \vec{\partial}_k u_{n,k}(\vec{r}')] e^{i\vec{k}\cdot\vec{r}} \} \\ &= \sum_n \int d\vec{k} \{ i \vec{\partial}_k \Psi_n(\vec{k}) \psi_{n,k}(\vec{r}) + \Psi_n(\vec{k}) \sum_m u_{m,k}(\vec{r}) [-\mathcal{A}_{mn}(k)] e^{i\vec{k}\cdot\vec{r}} \} \\ &= \sum_n \left[ \int d\vec{k} i \vec{\partial}_k \Psi_n(\vec{k}) \psi_{n,k}(\vec{r}) - \sum_m \vec{\mathcal{A}}_{m,n} \Psi_n(\vec{k}) \psi_{m,k}(\vec{r}) \right] \end{aligned} \quad (3.89)$$

If one only focus on a single band, say band n, we have

$$\vec{r} \Psi(\vec{r}) = \int d\vec{k} [i \vec{\partial}_k \Psi_n(\vec{k})] \psi_{n,k}(\vec{r}) - \int d\vec{r} \vec{\mathcal{A}}_{n,n} \Psi_n(\vec{r}) \psi_{n,k}(\vec{r}) \quad (3.90)$$

So:

$$\vec{r} = i \vec{\partial}_k - \vec{\mathcal{A}}_n \quad (3.91)$$

Just like what we are very familiar with for charged particles.

$$\vec{p} = -i \vec{\nabla}_x - \frac{e}{c} \vec{A} \quad (3.92)$$

More generic formula:

$$\vec{r} = i \vec{\partial}_k \delta_{n,m} - \vec{\mathcal{A}}_{m,n} \quad (3.93)$$

But we can usually ignore the terms  $m \neq n$  and they don't contribute to the Hall effect.

It is also worthwhile to notice that  $\vec{r} = i \vec{\nabla}_k - \vec{\mathcal{A}}_n$  is invariant under local phase change in the k-space  $|u_{n,k}\rangle \rightarrow e^{i\phi_n(k)} |u_{n,k}\rangle$ .

For a generic wavefunction, one can write as superpositions of Bloch waves

$$\Psi(\vec{r}) = \sum_n \int d\vec{k} \Psi_n(\vec{k}) \psi_{n,k}(\vec{r}) \quad (3.94)$$

The coefficient  $\Psi_n(\vec{k})$  is our wave-function. If we act  $(i \vec{\nabla}_k - \vec{\mathcal{A}}_n)$  on to  $\Psi_n(\vec{k})$ , and do the gauge transformation, one gets

$$\left( i \nabla_k - \vec{\mathcal{A}}_n \right) \Psi_n(\vec{k}) \rightarrow \left( i \nabla_k - \vec{\mathcal{A}}_n - \nabla_k \phi_n(k) \right) e^{-i \phi_n(k)} \Psi_n(\vec{k}) \quad (3.95)$$

Here we use the fact that under the gauge transformation,  $\psi_{n,k}(\vec{r}) \rightarrow e^{-i \phi_n(k)} \Psi_n(\vec{k})$ . To keep  $\Psi(\vec{r})$  invariant,  $\Psi_n(\vec{k}) \rightarrow e^{i \phi_n(k)} \Psi_n(\vec{k})$

$$\begin{aligned} \left( i \nabla_k - \vec{\mathcal{A}}_n \right) \psi_{n,k}(\vec{r}) &\rightarrow \left( i \nabla_k - \vec{\mathcal{A}}_n - \nabla_k \phi_n(k) \right) e^{-i \phi_n(k)} \Psi_n(\vec{k}) = \\ e^{i \phi_n(k)} \left( i \nabla_k - \vec{\mathcal{A}}_n - \nabla_k \phi_n(k) \right) \Psi_n(\vec{k}) &+ \nabla_k \phi_n(k) e^{i \phi_n(k)} \Psi_n(\vec{k}) = e^{i \phi_n(k)} \left( i \nabla_k - \vec{\mathcal{A}}_n \right) \Psi_n(\vec{k}) \end{aligned} \quad (3.96)$$

$$\Psi_n^*(\vec{k}) \left( i \nabla_k - \vec{\mathcal{A}}_n \right) \Psi_n(\vec{k}) \rightarrow e^{-i \phi_n(k)} \Psi_n^*(\vec{k}) e^{i \phi_n(k)} \left( i \nabla_k - \vec{\mathcal{A}}_n \right) \Psi_n(\vec{k}) = \Psi_n^*(\vec{k}) \left( i \nabla_k - \vec{\mathcal{A}}_n \right) \Psi_n(\vec{k}) \quad (3.97)$$

On the other hand, neither  $i \nabla_k$  nor  $\vec{\mathcal{A}}_n$  is invariant under this local phase change. So their value depends on the choice of gauge (choice of phases). This means that they are NOT physical observables and their value has no physics meaning. Only the sum of them two is meaningful, which is invariant under this “gauge transformation”.

### 3.6.4. Equations of motion and anomalous velocity

We know that under electric and magnetic fields (E and B), the equations of motion for a particle with charge  $e$  is

$$\frac{d\vec{p}}{dt} = \vec{F} = e \vec{E} + \frac{e}{c} \vec{v} \times \vec{B} = -e \vec{\nabla}_r \phi(r) + \frac{e}{c} \frac{d\vec{r}}{dt} \times [\vec{\nabla}_r \times \vec{A}(r)] \quad (3.98)$$

where  $\phi$  is the electric potential and  $A$  is the vector potential

In quantum mechanics,  $p$  and  $r$  are conjugate variables. We can choose to write the Hamiltonian as a function of  $r$  and  $\partial_r$ , or  $p$  and  $\partial_p$ . These two descriptions are equivalent. Since we can freely choose to use  $r$  or  $p$ , a natural question to ask is:

Q: What is the equations of motion for  $\vec{r}$ ? Is that EOM similar to the one shown above? Are there something like to  $\phi$  and  $\vec{A}$  in the E.O.M. for  $\vec{r}$

A: The EOM of  $\vec{r}$  looks almost identical to  $\vec{p}$ . We just need to switch  $r$  and  $p$ , and use the dispersion relation  $\epsilon(\vec{p})$  to replace  $\phi(\vec{r})$  and the Berry connection  $\vec{\mathcal{A}}(p)$  to replace the vector potential  $\vec{A}(\vec{r})$

$$\frac{d\vec{r}}{dt} = \nabla_p \epsilon(p) + \hbar \frac{d\vec{p}}{dt} \times [\vec{\nabla}_p \times \vec{\mathcal{A}}(p)] \quad (3.99)$$

For the special case of a free fermion with no E and B fields:  $\epsilon = p^2/2m$  and  $\vec{\mathcal{A}}(p)=0$ , this equation turns into

$$\frac{d\vec{r}}{dt} = \frac{\nabla_p p^2}{2m} = \frac{2\vec{p}}{2m} = \vec{v} \quad (3.100)$$

In many cases,  $\nabla_p \epsilon(p)$  is the definition of the “velocity” for a quantum particle. However, if  $\vec{\mathcal{A}}(p)$  is nonzero. This velocity is not just  $\nabla_p \epsilon(p)$ .

There is an extra term  $\frac{d\vec{p}}{dt} \times [\vec{\nabla}_p \times \vec{\mathcal{A}}(p)]$ , which is known as the “anomalous velocity”.

Let’s first go back to the EOM of  $\vec{p}$ . And demonstrate how this equation can be obtain in quantum mechanics.

the Hamiltonian is in general a function of  $r$  and  $p$ . In the real space, it is a function of  $\vec{r}$  and  $\vec{\partial}_r$ .

$$H = H(\vec{r}, \vec{p}) = H\left(\vec{r}, -i \hbar \vec{\partial}_r\right) \quad (3.101)$$

For charged particle, the momentum  $\vec{p}$  changes into  $\vec{p} = -i \hbar \vec{\partial}_r - \frac{e}{c} \vec{A}(r)$ . So the Hamiltonian is a function of  $\vec{r}$  and

$$H = H\left(\vec{r}, -i \hbar \vec{\partial}_r - \frac{e}{c} \vec{A}(r)\right) \quad (3.102)$$

In many cases, we can separate the Hamiltonian into a kinetic energy part and a potential energy part:

$$H = K(\vec{p}) + e\phi(\vec{r}) = K\left[-i\hbar\vec{\partial}_r - \frac{e}{c}\vec{A}(r)\right] + e\phi(\vec{r}) \quad (3.103)$$

Here  $K$  is the kinetic energy, which only depends on the momentum  $p$ . For charged particle,  $\vec{p} = -i\hbar\vec{\partial}_r - \frac{e}{c}\vec{A}(r)$ . The second term is the electric energy (potential energy), which only depends on  $\vec{r}$ .

Now, momentum  $\vec{p} = -i\hbar\vec{\partial}_r - \frac{e}{c}\vec{A}(r)$ , so

$$\begin{aligned} \frac{dp_i}{dt} &= \frac{i}{\hbar}[H, p_i] = \frac{i}{\hbar}\left[H, -i\hbar\partial_i - \frac{e}{c}A_i(r)\right] = [H, \partial_i] - \frac{i}{\hbar}\frac{e}{c}[H, A_i(r)] = \\ &= -\partial_{r_i}H - \frac{e}{c}\frac{d}{dt}A_i(\vec{r}) = -\partial_i K(\vec{p}) - e\partial_i\phi(\vec{r}) - \frac{e}{c}\frac{\partial A_i}{\partial r_j}\frac{dr_j}{dt} = -\frac{\partial K}{\partial p_j}\frac{\partial p_j}{\partial r_i} - e\partial_i\phi(\vec{r}) - \frac{e}{c}\frac{\partial A_i}{\partial r_j}\frac{dr_j}{dt} = \\ &= \frac{e}{c}\frac{\partial K}{\partial p_j}\frac{\partial A_j}{\partial r_i} - e\partial_i\phi(\vec{r}) - \frac{e}{c}\frac{\partial A_i}{\partial r_j}\frac{dr_j}{dt} = \frac{e}{c}\frac{\partial H}{\partial p_j}\frac{\partial A_j}{\partial r_i} - e\partial_i\phi(\vec{r}) - \frac{e}{c}\frac{\partial A_i}{\partial r_j}\frac{dr_j}{dt} = \\ &= \frac{e}{c}\frac{i}{\hbar}[H, r_j]\frac{\partial A_j}{\partial r_i} - e\partial_i\phi(\vec{r}) - \frac{e}{c}\frac{\partial A_i}{\partial r_j}\frac{dr_j}{dt} = \frac{e}{c}\frac{dr_j}{dt}\frac{\partial A_j}{\partial r_i} - e\partial_i\phi(\vec{r}) - \frac{e}{c}\frac{\partial A_i}{\partial r_j}\frac{dr_j}{dt} = -e\partial_i\phi(\vec{r})\frac{dr_j}{dt} + \\ &= \frac{e}{c}\frac{dr_j}{dt}\left(\frac{\partial A_j}{\partial r_i} - \frac{\partial A_i}{\partial r_j}\right) = -e\partial_i\phi(\vec{r})\frac{dr_j}{dt} + \frac{e}{c}v_j\left(\frac{\partial A_j}{\partial r_i} - \frac{\partial A_i}{\partial r_j}\right) = -e\partial_i\phi(\vec{r}) + \frac{e}{c}\left\{\frac{d\vec{r}}{dt} \times [\vec{\nabla}_r \times \vec{A}(r)]\right\}_i \end{aligned} \quad (3.104)$$

Now, let's go to the k-space

In a band theory, the Bloch waves are eigen-states of the Hamiltonian with dispersion relation  $\epsilon_n(k)$ . For simplicity, here we focus on one of the energy bands, so the Hamiltonian is

$$H = \epsilon_n(\vec{p}) \quad (3.105)$$

For charged particles,  $\vec{p} \rightarrow \vec{p} - \frac{e}{c}\vec{A}(\vec{r})$

$$H = \epsilon_n\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{r})\right) \quad (3.106)$$

So  $H$  is in general a function of  $\vec{p}$  and  $\vec{r}$ .

We know that for Bloch waves:  $\vec{r} = i\hbar\nabla_p - \vec{\mathcal{A}}_n$ . So

$$H = \mathcal{H}(\vec{p}, \vec{r}) = \mathcal{H}\left(\vec{p}, i\hbar\nabla_p - \vec{\mathcal{A}}_n\right) \quad (3.107)$$

This is almost the same as what we have above. So, if we follow the same steps, we find exactly the same equations of motion for  $\vec{r}$ .

$$\begin{aligned} \frac{dr_i}{dt} &= \frac{i}{\hbar}[H, r_i] = \frac{i}{\hbar}[H, i\hbar\partial_{p_i} - \mathcal{A}_i(p)] = \\ &= -[H, \partial_{p_i}] - \frac{i}{\hbar}[H, \mathcal{A}_i(p)] = \frac{d}{dp_i}\mathcal{H}(\vec{p}, \vec{r}) - \frac{i}{\hbar}[\mathcal{H}(\vec{p}, \vec{r}), \mathcal{A}_i(\vec{p})] = \partial_{p_i}\mathcal{H}(\vec{p}, \vec{r}) + \frac{\partial\mathcal{H}(\vec{p}, \vec{r})}{\partial r_j}\frac{\partial r_j}{\partial p_i} - \frac{d\mathcal{A}_i(\vec{p})}{dt} = \\ &= \partial_{p_i}\mathcal{H}(\vec{p}, \vec{r}) - \frac{\partial\mathcal{H}(\vec{p}, \vec{r})}{\partial r_j}\frac{\partial\mathcal{A}_j}{\partial p_i} - \frac{\partial\mathcal{A}_i(\vec{p})}{\partial p_j}\frac{dp_j}{dt} = \partial_{p_i}\mathcal{H}(\vec{p}, \vec{r}) + \frac{dp_j}{dt}\frac{\partial\mathcal{A}_j}{\partial p_i} - \frac{\partial\mathcal{A}_i}{\partial p_j}\frac{dp_j}{dt} \end{aligned} \quad (3.108)$$

Here we used that

$$\frac{\partial\mathcal{H}(\vec{p}, \vec{r})}{\partial r_j} = -\frac{i}{\hbar}[\mathcal{H}(\vec{p}, \vec{r}), p_j] = -\frac{dp_j}{dt} \quad (3.109)$$

So

$$\frac{d r_i}{d t} = \partial_{p_i} \mathcal{H}(\vec{k}, \vec{r}) + \frac{d p_j}{d t} \left( \frac{\partial \mathcal{A}_j}{\partial p_i} - \frac{\partial \mathcal{A}_i}{\partial p_j} \right) \quad (3.110)$$

In the weak field limit,

$$H = \epsilon_n \left( \vec{p} - \frac{e}{c} \vec{A}(\vec{r}) \right) \approx \epsilon_n(p) \quad (3.111)$$

So

$$\frac{d r_i}{d t} = \partial_{p_i} \mathcal{H}(\vec{p}, \vec{r}) + \frac{d p_j}{d t} \left( \frac{\partial \mathcal{A}_j}{\partial p_i} - \frac{\partial \mathcal{A}_i}{\partial p_j} \right) \approx \partial_{p_i} \epsilon_n + \frac{d p_j}{d t} \left( \frac{\partial \mathcal{A}_j}{\partial p_i} - \frac{\partial \mathcal{A}_i}{\partial p_j} \right) \quad (3.112)$$

$$\frac{d \vec{r}}{d t} = \nabla_p \epsilon(p) + \frac{d \vec{p}}{d t} \times \left[ \nabla_p \times \vec{\mathcal{A}}(p) \right] \quad (3.113)$$

### 3.6.5. Berry curvature and the Hall effect

Reference: Haldane, Berry Curvature on the Fermi Surface: Anomalous Hall Effect as a Topological Fermi-Liquid Property, Phys. Rev. Lett. 93, 206602 (2004).

In the presence of  $E$  and  $B$  fields, the Newton's second law reads

$$\frac{d \vec{p}}{d t} = \vec{F} = e \vec{E} + e \vec{v} \times \vec{B} \quad (3.114)$$

$$\frac{d \vec{r}}{d t} = \nabla_p \epsilon(p) + \frac{d \vec{p}}{d t} \times \left[ \nabla_p \times \vec{\mathcal{A}}(p) \right] \quad (3.115)$$

If all the electrons have the same velocity, we have current:

$$j = e n v = \frac{e N v}{A} \quad (3.116)$$

If the velocities are different,

$$j = \frac{e}{A} \sum_m v_m = \frac{e}{A} \sum_m \frac{d r_m}{d t} = e \sum_{\text{fully occupied bands}} \frac{A}{h^2} \int_{\text{BZ}} d \vec{p} \left\{ \nabla_p \epsilon_n(p) + \frac{d \vec{p}}{d t} \times \left[ \nabla_p \times \vec{\mathcal{A}}_n(p) \right] \right\} + e \sum_{\text{partially filled bands}} \frac{A}{h^2} \int_{\text{occupied part}} d \vec{p} \left\{ \nabla_p \epsilon_n(p) + \frac{d \vec{p}}{d t} \times \left[ \nabla_p \times \vec{\mathcal{A}}_n(p) \right] \right\} \quad (3.117)$$

For an insulator, we only have fully filled bands so we can drop the last term.

$$\frac{d \vec{r}}{d t} = \nabla_p \epsilon_n(p) + \frac{d \vec{p}}{d t} \times \left[ \nabla_p \times \vec{\mathcal{A}}_n(p) \right] = \nabla_p \epsilon_n(p) + \left( e \vec{E} + e \vec{v} \times \vec{B} \right) \times \left[ \nabla_p \times \vec{\mathcal{A}}_n(p) \right] \quad (3.118)$$

Here, one term is important:

$$e \vec{E} \times \left[ \nabla_p \times \vec{\mathcal{A}}_n(p) \right] \quad (3.119)$$

If we changes all the  $p$  back to  $k$ , we get one extra  $\hbar$

$$e \vec{E} \times \left[ \nabla_p \times \vec{\mathcal{A}}_n(p) \right] = \frac{1}{\hbar} e \vec{E} \times \left[ \nabla_k \times \vec{\mathcal{A}}_n(k) \right] \quad (3.120)$$

In addition,  $\int d p$  turns into  $\hbar^2 \int d k$

This one gives Hall effect: velocity of the electron is perpendicular to the direction of  $\vec{E}$ . So if we only care about Hall conductivity, the Hall current is



$$j_H = \frac{e^2}{2\pi\hbar} \sum_{n \text{ fully occupied bands}} \int_{\text{BZ}} d\vec{k} \vec{E} \times \left[ \vec{\nabla}_k \times \vec{\mathcal{A}}_n(k) \right] = \vec{E} \times \left[ \frac{e^2}{\hbar} \frac{1}{2\pi} \sum_{n \text{ fully occupied bands}} \int_{\text{BZ}} d\vec{k} \vec{E} \times \vec{\mathcal{F}}_n(k) \right] \quad (3.121)$$

$$\sigma_{xy} = \frac{e^2}{\hbar} \sum_{n \text{ fully occupied bands}} \left[ \frac{1}{2\pi} \int_{\text{BZ}} d\vec{k} \vec{\mathcal{F}}_n(k) \right] \quad (3.122)$$

In the next section, we will show that the integral here is always an integer, and it is a topological index.

From now on, I will use the theorist's unit:  $k_B = e = c = \hbar = 2\pi = 1$  so

$$\sigma_{xy} = \sum_n \left[ -\frac{i}{2\pi} \int_{\text{BZ}} d\vec{k} \epsilon_{ij} \langle \partial_{ki} u_{n,k} | \partial_{kj} u_{n,k} \rangle \right] \quad (3.123)$$

is just an integer.

### 3.7. Dirac Quantization, Gauss–Bonnet theorem and the TKNN (Thouless —Kohmoto —Nightingale —den Nijs ) Invariant

From the mathematical point of the view, the following three objects are the same thing (fiber bundles): the magnetic field  $B$ , the Berry curvature  $\mathcal{F}$ , and the Gaussian curvature of  $K$  (geometry). All of them are described by the same mathematical structure: fiber bundles.

In the next a few sections, we will investigate the integral of  $B$ ,  $\mathcal{F}$  and  $K$  on a closed 2D manifold. (close: no boundary). And shows that they are all quantized due to topological reasons, which is known as topological quantization.

$$\oint_M B \cdot dS = \oint_M B_n dS = \frac{c\hbar}{2q_e} n \quad \text{quantized : } n \text{ is an integer,} \quad (3.124)$$

known as the magnetic charge, which measures the number of magnetic monopole inside  $M$

$$\oint_M K dS = 2\pi \chi_M \quad \text{quantized : } \chi_M \text{ is an even integer,} \quad (3.125)$$

known as the Euler characteristic, which measures the topological nature of the manifold  $M$

$$\oint_{\text{BZ}} \mathcal{F} d\vec{k} = 2\pi C \quad \text{quantized : } C \text{ is an integer,} \quad (3.126)$$

known as the TKNN invariant or the Chern number, which measures the quantized Hall conductivity for a topological insulator

### 3.8. Magnetic monopole and Dirac quantization condition

Reference: M Nakahara, Geometry, topology and physics, IOP

For electric charge, the Gauss's law tell us that

$$q_e = \oint_M E \cdot dS \quad (3.127)$$

In Maxwell's equations, this is:

$$\nabla \cdot E = \rho \quad (3.128)$$

For magnetic fields, we can do the same thing:

$$q_m = \oint_M B \cdot dS \quad (3.129)$$

Without magnetic monopoles,  $q_m = 0$ , because  $\nabla \cdot B = 0$

Assume that there is a magnetic monopole with charge  $q_m$ , what will happen?

The  $B$  fields is: