

Examples: If one comb the hair along the longitude (or latitude) directions, there are two +1 vortex at north and south poles.

If one assumes that human hair covers the north hemisphere (of the head) and pointing downward (to -z) at the equator, which is typically true for human hairs, vorticity total is +1 (half of +2). For the majority of human beings, there is one +1 vortex. But there are more complicated cases, for example two +1 and one -1, or three +1 and two -1.

### 3.10. Topological index for an insulator

The topological index

$$C = \frac{1}{2\pi} \sum_n \oint_{\text{BZ}} \mathcal{F} d\vec{k} \quad (3.164)$$

This integral is a topological index only if we integrate  $\mathcal{F}$  over the whole BZ (a closed manifold). Because a BZ has periodic boundary conditions along x and y (for a 2D system), the BZ is a torus which is a closed manifold.

$$\mathcal{F}_n(\vec{k}) = \epsilon_{ij} \langle \partial_{k_i} u_{n,k} | \partial_{k_j} u_{n,k} \rangle \quad (3.165)$$

$$\sigma_{xy} = \frac{e^2}{h} \sum_{n, \text{valence bands}} \left[ \frac{1}{2\pi} \int_{\text{BZ}} d\vec{k} \mathcal{F}_n(\vec{k}) \right] + \frac{e^2}{h} \sum_{n, \text{conduction bands}} \left[ \frac{1}{2\pi} \int_{\epsilon_k < \epsilon_F} d\vec{k} \mathcal{F}_n(\vec{k}) \right] \quad (3.166)$$

For 2D systems, we will show below that the first term is quantized and is topologically invariant. The second term is not quantized and is not topologically invariant.

For insulators (first term only), the Hall conductivity is a topological index and is an Integer due to topological quantization.

For metals, the integral for the conducting band is taken over only part of the BZ (the filled states, or say the Fermi sea). It is not quantized and it is not a topological index.

In other words,  $\mathcal{F}$  gives us 2D topological insulators, but no topological metals.

### 3.11. Second quantization

#### 3.11.1. wave functions for indistinguishable particles

Second quantization is a technique to handle indistinguishable particles.

Two distinguishable particles: particle one on state  $\psi_1$  and particle two on state  $\psi_2$

$$\Psi(r_1, r_2) = \psi_1(r_1) \psi_2(r_2) \quad (3.167)$$

n distinguishable particles:

$$\Psi(r_1, r_2, r_3, \dots, r_n) = \psi_1(r_1) \psi_2(r_2) \dots \psi_n(r_n) \quad (3.168)$$

Two indistinguishable particles: particle one on state  $\psi_1$  and particle two on state  $\psi_2$

$$\Psi(r_1, r_2) = \pm \Psi(r_2, r_1) \quad (3.169)$$

$$\Psi(r_1, r_2) = \psi_1(r_1) \psi_2(r_2) \pm \psi_2(r_1) \psi_1(r_2) \quad (3.170)$$

3 indistinguishable particles:

$$\begin{aligned} \Psi(r_1, r_2, r_3) = & \psi_1(r_1) \psi_2(r_2) \psi_3(r_3) \pm \psi_1(r_1) \psi_3(r_3) \psi_2(r_2) \pm \psi_2(r_2) \psi_1(r_1) \psi_3(r_3) + \\ & \psi_3(r_3) \psi_1(r_1) \psi_2(r_2) + \psi_2(r_2) \psi_3(r_3) \psi_1(r_1) \pm \psi_3(r_3) \psi_2(r_2) \psi_1(r_1) \end{aligned} \quad (3.171)$$

n indistinguishable particles:

$$\Psi(r_1, r_2, r_3, \dots, r_n) = \sum_{\mathcal{P}} (\pm 1)^{\mathcal{P}} \psi_{i_1}(r_1) \psi_{i_2}(r_2) \dots \psi_{i_n}(r_n) \quad (3.172)$$

where  $\mathcal{P}$  represents all permutations and there are n! terms here. For large n, this is an extremely complicated wavefunction. For even ten particles, n=10, there are 2.6 million terms.

### 3.11.2. Fock space

The problem here is because Schrodinger equations and wavefunctions are designed for distinguishable particles and one needs to symmetries or anti-symmetries all the wavefunctions by hand.

For indistinguishable particles, it is more natural to use the particle number basis, the Fock space. In the Fock space, the many-body quantum state are written in terms of occupation numbers:

$$|\Psi\rangle = |n_1, n_2, n_3 \dots n_N\rangle \quad (3.173)$$

where  $n_i$  is the number of particles in state  $|\psi_i\rangle$ . Here we don't specify which particle is in the state  $|\psi_i\rangle$ , only count the number of particles on this state, which makes the particle indistinguishable automatically.

### 3.11.3. Creation and annihilation operators:

In the Fock space, all physical operators can be written in terms of creation and annihilation operators:

For bosons

$$b_i^\dagger |n_1, n_2, n_3 \dots n_N\rangle = \sqrt{n_i + 1} |n_1, n_2, \dots, n_i + 1, \dots, n_N\rangle \quad (3.174)$$

$$b_i |n_1, n_2, n_3 \dots n_N\rangle = \sqrt{n_i} |n_1, n_2, \dots, n_i - 1, \dots, n_N\rangle \quad (3.175)$$

$$[b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0 \quad (3.176)$$

$$[b_i, b_j^\dagger] = \delta_{ij} \quad (3.177)$$

For fermions  $n_i = \pm 1$  (Pauli exclusive principle)

$$c_i^\dagger | \dots, 1, \dots \rangle = 0 \quad (3.178)$$

$$c_i^\dagger | \dots, 0, \dots \rangle = | \dots, 1, \dots \rangle \quad (3.179)$$

$$c_i | \dots, 1, \dots \rangle = 0 \quad (3.180)$$

$$c_i | \dots, 0, \dots \rangle = | \dots, 0, \dots \rangle \quad (3.181)$$

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0 \quad (3.182)$$

$$\{c_i, c_j^\dagger\} = \delta_{ij} \quad (3.183)$$

### 3.11.4. Particle number operator

Particle number operator for bosons  $n_i = b_i^\dagger b_i$

$$b_i^\dagger b_i | \dots, n_i, \dots \rangle = n_i | \dots, n_i, \dots \rangle \quad (3.184)$$

Total particle number  $N = \sum_i n_i = \sum_i b_i^\dagger b_i$

Particle number operator for fermions  $n_i = c_i^\dagger c_i$

$$c_i^\dagger c_i | \dots, 0, \dots \rangle = 0 \quad (3.185)$$

$$c_i^\dagger c_i | \dots, 1, \dots \rangle = 1 | \dots, 1, \dots \rangle \quad (3.186)$$

Total particle number  $N = \sum_i n_i = \sum_i c_i^\dagger c_i$

### 3.11.5. Quantum states

In the Fock space, all quantum states can be written in terms of creation and annihilation operators:

Vacuum (ground states in high energy physics)  $|G\rangle$ . We assume that there is one and only one state in the Fock space that is annihilated by any annihilation operators. This is our vacuum state.

$$c_i | G \rangle = 0 \text{ for any } c_i \quad (3.187)$$

one particle states

$$\psi = \sum_e a_i c_i^\dagger | G \rangle \quad (3.188)$$

two particle states

$$\psi = \sum_{ij} a_{ij} c_j^\dagger c_i^\dagger | G \rangle \quad (3.189)$$

n particle states

$$\psi = \sum_{i_1 \dots i_n} a_{i_1 \dots i_n} c_{i_n}^\dagger \dots c_{i_2}^\dagger c_{i_1}^\dagger | G \rangle \quad (3.190)$$

### 3.11.6. Physical observables and expectation values

All physical observables can be written in terms of expectation values for these creation and annihilation operators:

$$X = \langle \Psi | X | \Psi \rangle = \sum_{i_1, \dots, i_N} \langle G | c_{i_1} \dots c_{i_n} c_{i_n}^\dagger \dots c_{i_2}^\dagger c_{i_1}^\dagger | G \rangle \quad (3.191)$$

Remarks: these procedures are known as the “Second Quantization”

- This name are used due to historical reasons. We are not quantizing something once again. We are just using a new basis to handle indistinguishable particles.
- It is just one step away from quantum field theory. (will be discussed later)
- In both high energy and condensed matter physics, quantum field theory utilize the “Second Quantization” construction. The reason is because quantum field theory deals with more than one indistinguishable palaces, and the Second Quantization formulas are the most natural way to describe this time of physics.

## 3.12. tight-binding models

Fermions hopping on a lattice and each lattice site can only have n discrete quantum state. It is an simplified model for relay crystals (a discretize version of a metal). It captures most of the essential physics and provides the same physics phenomena.

One unit cell main contain multi sites (multi atoms in a unit cell), saying m sites. A site are marked by two numbers the unit cell index  $i=1, 2, \dots, N$  and the site index  $\alpha=1, 2, 3, \dots, m$

Coordinate of a site: for site  $(i, \alpha)$  the position is  $x = i a + r_\alpha$

Bloch wave:

$$\psi_{n,k}(x) = u_{n,k}(x) e^{i k x} \quad \text{continues models} \quad (3.192)$$

$$\psi_{n,j,\alpha}(k) = u_{n,\alpha}(k) \frac{e^{i k x}}{\sqrt{2 \pi / a}} \quad \text{tight - binding models} \quad (3.193)$$

Find the Bloch wave function = find  $u_{n,\alpha}$

Berry connection and Berry curvature:

$$\mathcal{A}_{n,k} = -i \langle u_{n,k} | \partial_k | u_{n,k} \rangle = -i \int dx u_{n,k}^*(r) \partial_k u_{n,k}(r) = -i \sum_{\alpha} u_{n,\alpha}(k)^* \partial_k u_{n,\alpha}(k) \quad (3.194)$$

$$\mathcal{F}_{n,k} = -i \epsilon_{ij} \langle \partial_{k_i} u_{n,k} | \partial_{k_j} u_{n,k} \rangle = -i \epsilon_{ij} \int dx \partial_{k_i} u_{n,k}^*(r) \partial_{k_j} u_{n,k}(r) = -i \epsilon_{ij} \sum_{\alpha} \partial_{k_i} u_{n,\alpha}(k)^* \partial_{k_j} u_{n,\alpha}(k) \quad (3.195)$$

### 3.12.1. Example: a one-band model

Lets consider a simple 1D lattice with only one type of atoms.

$$H = - \sum_{ij} (t_{ij} c_i^\dagger c_j + t_{ij}^* c_j^\dagger c_i) + \sum_e V_i c_i^\dagger c_i \quad (3.196)$$

The first term describes the hopping from site j to i and the second term describes the hopping from i to j. Because  $H$  is Hermitian, the two coefficients must be equal to each other. Because the lattice contains only one type of atoms,  $V_i = \text{constant}$

$$H = -\sum_{ij} (t_{ij} c_i^\dagger c_j + t_{ij}^* c_j^\dagger c_i) + V \sum_i c_i^\dagger c_i = -\sum_{ij} (t_{ij} c_i^\dagger c_j + t_{ij}^* c_j^\dagger c_i) + V N \quad (3.197)$$

The last term  $V N$  is a constant. It shift the total energy by a constant, and has no other physical contribution (can be ignored if we are not interested in the total energy). In addition, we assume the electrons can only hop to the nearest neighbor: Due to translational symmetry, for all NN hoppings, the  $t$  must be the same. If we assume  $t$  is real (which is always the case for 1D NN hopping-only models)

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) = -t \sum_i c_i^\dagger c_{i+1} + h.c. \quad (3.198)$$

Fourier series:

Typically, Fourier series are applied to a periodic function in the real space, which will have a describe set of wavevectors in the  $k$  space. Here, it is the opposite. We have a continuous  $k$ -space and it is periodic (BZ), but the real space is discrete.

$$c_k = \frac{\sqrt{a}}{\sqrt{2\pi}} \sum_i c_i e^{-ikx} \quad (3.199)$$

$$c_i = \frac{\sqrt{a}}{\sqrt{2\pi}} \int_{\text{BZ}} dk c_k e^{ikx} \quad (3.200)$$

$$\{c_k, c_{k'}^\dagger\} = \left\{ \frac{1}{\sqrt{2\pi/a}} \sum_i c_i e^{-ikx_i}, \frac{1}{\sqrt{2\pi/a}} \sum_j c_j^\dagger e^{ik'x_j} \right\} = \quad (3.201)$$

$$\sum_{i,j} \{c_i, c_j^\dagger\} \frac{1}{2\pi/a} e^{-ikx_i} e^{ik'x_j} = \sum_{i,j} \delta_{i,j} \frac{1}{2\pi/a} e^{-i(k-k')x_i} = \sum_i \frac{1}{2\pi/a} e^{-i(k-k')ia} = a \delta((k-k')a) = \delta(k-k')$$

$$\{c_i, c_j^\dagger\} = \left\{ \frac{1}{\sqrt{2\pi/a}} \int_{\text{BZ}} dk c_k e^{ikx_i}, \frac{1}{\sqrt{2\pi/a}} \int_{\text{BZ}} dk' c_{k'}^\dagger e^{-ik'x_j} \right\} = \quad (3.202)$$

$$\frac{1}{2\pi/a} \int_{\text{BZ}} dk \int_{\text{BZ}} dk' \{c_k, c_{k'}^\dagger\} e^{ikx_i} e^{-ik'x_j} = \frac{1}{2\pi/a} \int_{\text{BZ}} dk \int_{\text{BZ}} dk' \delta(k-k') e^{ikx_i} e^{-ik'x_j} = \frac{1}{2\pi/a} \int_{\text{BZ}} dk e^{ik(x_i-x_j)} = \delta_{ij}$$

The Hamiltonian:

$$H = -t \sum_i c_i^\dagger c_{i+1} + h.c. \quad (3.203)$$

$$\sum_j c_j^\dagger c_{j+1} = \sum_j \frac{1}{\sqrt{2\pi/a}} \int_{\text{BZ}} dk c_k^\dagger e^{-ikaj} \frac{1}{\sqrt{2\pi/a}} \int_{\text{BZ}} dk' c_{k'} e^{ik'(j+1)a} = \quad (3.204)$$

$$\sum_j \frac{1}{2\pi/a} \int_{\text{BZ}} dk \int_{\text{BZ}} dk' c_k^\dagger c_{k'} e^{ik'aj} e^{-i(k-k')aj} = \int_{\text{BZ}} dk \int_{\text{BZ}} dk' c_k^\dagger c_{k'} \delta(k-k') = \int_{\text{BZ}} dk c_k^\dagger c_k e^{ikaj}$$

$$H = -t \sum_i c_i^\dagger c_{i+1} + h.c. = -t \int_{\text{BZ}} dk c_k^\dagger c_k e^{ikaj} + h.c. = \quad (3.205)$$

$$-t \int_{\text{BZ}} dk c_k^\dagger c_k e^{ikaj} - t \int_{\text{BZ}} dk c_k^\dagger c_k e^{-ikaj} = -2t \int_{\text{BZ}} dk c_k^\dagger c_k \cos ka = \int_{\text{BZ}} dk (-2t \cos ka) n_k$$

$$E = \int dk \epsilon_k n_k \quad (3.206)$$

Dispersion relation:

$$\epsilon_k = -2t \cos ka \quad (3.207)$$

$\epsilon_k$  is a periodic function of  $k$ . However, we only have one band.

Bloch wave:

$$\psi_n(k) = u_{n,\alpha}(k) \frac{e^{ikx}}{\sqrt{2\pi/a}} \quad (3.208)$$