

Condensed Matter Physics

Part 2. Electronic System

Electrons in Solids

■ Quantum Mechanics of Electrons

■ Schrödinger Equation of Electron

An **electron** is a quantum particle described by the **Schrödinger equation**

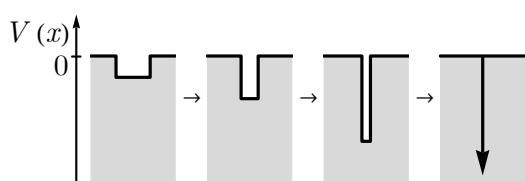
$$\left(-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{x}) \right) \psi(\mathbf{x}) = E \psi(\mathbf{x}). \quad (1)$$

- m - electron **mass**,
- $V(\mathbf{x})$ - electronic **potential** at position \mathbf{x} ,
- $\psi(\mathbf{x})$ - electron **wave function** (eigenstate), s.t. the *probability* (density) to observe an electron at position \mathbf{x} is $|\psi(\mathbf{x})|^2$,
- E - the corresponding eigen **energy** of the eigenstate.

■ A Toy Atom in 1D

Consider an electron in 1D. An atomic **nucleus** (or a positively-charged ion) at the origin can be modeled by an *attractive Dirac potential* (with $-\gamma < 0$)

$$V(x) = -\gamma \delta(x), \quad (2)$$



The Dirac potential viewed as the *limit* of square potential wells, where the potential is infinitely *narrow* and infinitely *deep* but keeps the width \times depth = γ constant. The constant γ effectively describes the *strength* of the potential (which has to do with the nucleus charge etc.).

Schrödinger equation

$$-\frac{\hbar^2}{2m} \partial_x^2 \psi(x) - \gamma \delta(x) \psi(x) = E \psi(x). \quad (3)$$

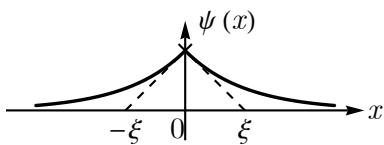
- **Bound state ($E < 0$)**

- Wave function decays *exponentially* near the origin,

$$\psi(x) = \xi^{-1/2} e^{-|x|/\xi}, \quad (4)$$

with a decay length

$$\xi = \frac{\hbar^2}{m\gamma}. \quad (5)$$



In the *bound state*, the electron is *trapped* around the potential within the *length scale* ξ . \Rightarrow The model mimics an **atom** (in 1D), where ξ can be viewed as the **atomic radius** (Bohr radius).

- The **eigen energy** is *negative* (with respect to the potential zero)

$$E = -\frac{\hbar^2}{2m\xi^2} = -\frac{m\gamma^2}{2\hbar^2}. \quad (6)$$

- This is the *unique* bound state in the system, which is also the lowest-energy **ground state** of the electron.

Exc 1 Verify that Eq. (4) is a normalized solution of Eq. (3).

- **Scattering states ($E > 0$)**

- There are infinitely many scattering state solutions (forming a continuum in the spectrum). Each scattering state is associated with an *positive* **eigen energy** $E > 0$, which also sets a **wave number**

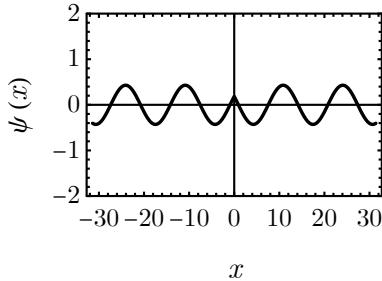
$$k = \frac{\sqrt{2mE}}{\hbar}. \quad (14)$$

- Wave function

$$\psi(x) = \begin{cases} e^{ikx} + A_r e^{-ikx} & x < 0 \\ A_t e^{ikx} & x > 0 \end{cases}, \quad (15)$$

with the *reflection* and *transmission* amplitudes

$$\begin{aligned} A_r &= -\frac{1}{1 + i k \xi}, \\ A_t &= \frac{1}{1 - i / (k \xi)}. \end{aligned} \quad (16)$$



- In the *scattering state*, the electron has high enough energy to scatter off the potential. \Rightarrow The atom **ionize** into dissociated electron and nucleus.
- In the following, we will be interested in bound states of electrons (in atomic orbitals), which are relevant to the solid state physics.

■ Two Toy Atoms in 1D

Place two nuclei from each other by distance d . An electron will experience two attractive Dirac potentials

$$V(x) = -\gamma \delta(x - d/2) - \gamma \delta(x + d/2). \quad (17)$$

Define the atomic radius

$$\xi = \frac{\hbar^2}{m \gamma}. \quad (18)$$

- Bound state ($E < 0$) wave functions

- Even parity solution

$$\psi(x) = \begin{cases} A e^{\kappa x} & x < -d/2, \\ \cosh \kappa x & -d/2 < x < d/2, \\ A e^{-\kappa x} & x > d/2. \end{cases} \quad (19)$$

- Odd parity solution

$$\psi(x) = \begin{cases} -A e^{\kappa x} & x < -d/2, \\ \sinh \kappa x & -d/2 < x < d/2, \\ A e^{-\kappa x} & x > d/2. \end{cases} \quad (20)$$

- The amplitude A is given by (continuity of wave function)

$$A = \begin{cases} \frac{1}{2} (e^{\kappa d} + 1) & \text{even parity,} \\ \frac{1}{2} (e^{\kappa d} - 1) & \text{odd parity.} \end{cases} \quad (21)$$

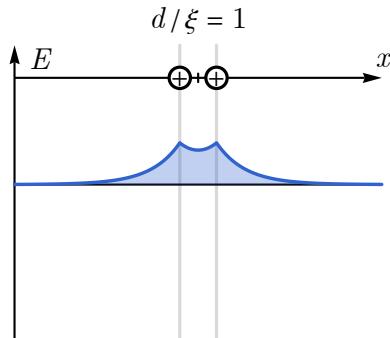
- Substitute Eq. (19), Eq. (20) into the Schrödinger equation, the imaginary wave number κ is determined by

$$e^{\kappa d}(\kappa \xi - 1) = \begin{cases} +1 & \text{even parity,} \\ -1 & \text{odd parity,} \end{cases} \quad (22)$$

Exc 2 | Derive Eq. (22).

The number of solutions of Eq. (22) depends on the inter-atomic distance d and the atomic radius ξ ,

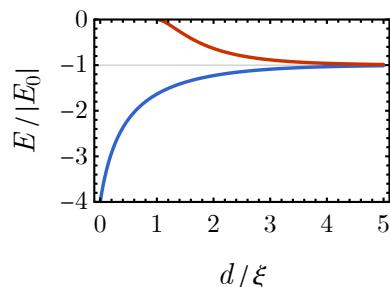
- $d > \xi$: two bound states of both parities,
- $d < \xi$: one bound state of even parity.



- : even parity solution,
- : odd parity solution.

- Based on the solutions of κ , the eigen energies are given by

$$E = -\frac{\hbar^2 \kappa^2}{2 m}. \quad (39)$$



- The energy E is plotted in unit of the ground state energy E_0 of a single atom given in Eq. (6)

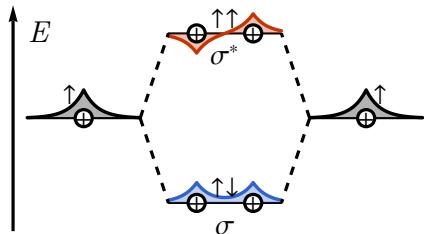
$$E_0 = -\frac{\hbar^2}{2 m \xi^2}. \quad (40)$$

- The *even* parity state is always the *ground state* of the two-atom system.
- Assuming electrons always occupy the ground state, as the atoms merge together (from $d \rightarrow \infty$ to $d \rightarrow 0$), the **binding energy** $E_b = E_{d \rightarrow \infty} - E_{d=0} = 3 |E_0|$ will be released (per electron).
- Force** between atoms are given by

$$F = -\frac{\partial E}{\partial d} \quad (41)$$

Inter-atomic force can be *mediated* by *exchanging* electron \Rightarrow **valence bond**.

- Molecular orbitals** of valence σ -bond



- Bonding orbital:** electron in *even* parity state, atoms *attract* each other.
- Anti-bonding orbital:** electron in *odd* parity state, atoms *repel* each other.

■ Tight Binding Approximation

Tight binding (atomic) limit: When the inter-atomic distance d is sufficiently large compared to the atomic radius ξ (i.e. $d \gg \xi$) \Rightarrow the electron tightly binds the atomic nucleus, such that the molecular orbital can be *approximated* by superpositions of atomic orbitals.

- Atomic orbitals**

$$\langle x|1\rangle = \psi_1(x) = \xi^{-1/2} e^{-|x-x_1|/\xi},$$

$$\langle x|2\rangle = \psi_2(x) = \xi^{-1/2} e^{-|x-x_2|/\xi}, \quad (42)$$

where x_1 and x_2 are the positions of two nuclei respectively.

- $|1\rangle$ and $|2\rangle$ are not orthogonal, but close to orthogonal in the tight binding limit

$$\begin{aligned} \langle 1|2\rangle &= \int_{-\infty}^{\infty} \psi_1^*(x) \psi_2(x) dx \\ &= \xi^{-1} \int_{-\infty}^{\infty} e^{-|x-x_1|/\xi} e^{-|x-x_2|/\xi} dx \end{aligned} \quad (43)$$

$$= e^{-d/\xi} (1 + d/\xi) \xrightarrow{d \gg \xi} 0,$$

where $d = |x_1 - x_2|$.

- **Tight binding basis:** *orthogonalized atomic orbitals*

$$|\tilde{i}\rangle = \sum_i S_{i\tilde{i}} |i\rangle,$$

(44)

such that $\langle \tilde{i} | \tilde{j} \rangle = \delta_{ij}$.

- The transformation matrix is given by

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \sqrt{\cosh 2\varepsilon} \begin{pmatrix} \cosh \varepsilon & -\sinh \varepsilon \\ -\sinh \varepsilon & \cosh \varepsilon \end{pmatrix}. \quad (45)$$

where ε is defined by

$$\tanh 2\varepsilon = e^{-d/\xi} (1 + d/\xi). \quad (46)$$

- ε is expected to vanish in the tight binding limit. To the leading order in ε ,

$$\begin{aligned} |\tilde{1}\rangle &\simeq |1\rangle - \varepsilon |2\rangle, \\ |\tilde{2}\rangle &\simeq |2\rangle - \varepsilon |1\rangle, \end{aligned} \quad (47)$$

with $\varepsilon \simeq \frac{1}{2} e^{-d/\xi} (1 + d/\xi)$.

- Hamiltonian operator

$$\begin{aligned} H &= -\frac{\hbar^2}{2m} \partial_x^2 + V(x) \\ &= -\frac{\hbar^2}{2m} \partial_x^2 - \gamma \delta(x - x_1) - \gamma \delta(x - x_2). \end{aligned} \quad (48)$$

It is assumed that γ and ξ are always related by $\xi = \hbar^2 / (m\gamma)$, such that $|1\rangle$ and $|2\rangle$ are eigenstates of the Hamiltonian when only one potential is present, i.e.

$$\left(-\frac{\hbar^2}{2m} \partial_x^2 - \gamma \delta(x - x_i) \right) \psi_i(x) = E_0 \psi_i(x), \quad (49)$$

with the atomic orbital eigen energy

$$E_0 = -\frac{\hbar^2}{2m\xi^2}.$$

(50)

- **Tight binding Hamiltonian:** the effective Hamiltonian in the tight binding basis

$$H_{\text{eff}} = \sum_{i,j=1,2} |\tilde{i}\rangle \tilde{H}_{ij} \langle \tilde{j}|, \quad (51)$$

where $\tilde{H}_{ij} \equiv \langle \tilde{i} | H | \tilde{j} \rangle$.

- The matrix element \tilde{H}_{ij} can be obtained from

$$\begin{aligned} H_{ij} &\equiv \langle i | H | j \rangle \\ &= \int_{-\infty}^{\infty} \psi_i^*(x) \left(-\frac{\hbar^2}{2m} \partial_x^2 - \gamma \delta(x - x_1) - \gamma \delta(x - x_2) \right) \psi_j(x) dx, \end{aligned} \quad (52)$$

via basis transformation Eq. (44)

$$\tilde{H}_{ij} = \sum_{ij} S_{\tilde{i}i} H_{ij} S_{\tilde{j}j}, \quad (53)$$

or written in terms of matrix multiplication $\tilde{H} = S H S^T$.

- Substitute Eq. (42) into Eq. (52), one finds

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} = E_0 \begin{pmatrix} 1 + 2e^{-2d/\xi} & e^{-d/\xi}(3 + d/\xi) \\ e^{-d/\xi}(3 + d/\xi) & 1 + 2e^{-2d/\xi} \end{pmatrix}, \quad (54)$$

where E_0 is the atomic orbital energy.

**Exc
3**

Derive Eq. (54).

- Substitute Eq. (45) and Eq. (54) into Eq. (53), to the leading order of $e^{-d/\xi}$ (in the tight binding limit), the effective Hamiltonian reads

$$\begin{aligned} \tilde{H} &= S H S^T \\ &= E_0 \begin{pmatrix} 1 & 2e^{-d/\xi} \\ 2e^{-d/\xi} & 1 \end{pmatrix} + O(e^{-2d/\xi}). \end{aligned} \quad (60)$$

or written in the tight binding basis as

$$H_{\text{eff}} = E_0(|\tilde{1}\rangle\langle\tilde{1}| + |\tilde{2}\rangle\langle\tilde{2}|) + 2E_0e^{-d/\xi}(|\tilde{1}\rangle\langle\tilde{2}| + |\tilde{2}\rangle\langle\tilde{1}|). \quad (61)$$

- The diagonal term $|\tilde{1}\rangle\langle\tilde{1}| + |\tilde{2}\rangle\langle\tilde{2}|$ describes that the electron trapped around an atom will experience the **on-site energy** E_0 .
- The off-diagonal term $|\tilde{1}\rangle\langle\tilde{2}| + |\tilde{2}\rangle\langle\tilde{1}|$ describes that the electron can tunnel from one atom to another, and the process is associated with an energy scale $2E_0e^{-d/\xi}$, which is also called the **hopping energy**.
- **Molecular orbitals** (tight binding model)

- In the tight binding basis, the Schrödinger equation reduces from a differential equation to a matrix equation

$$H_{\text{eff}} |\psi\rangle = E |\psi\rangle, \quad (62)$$

or explicitly

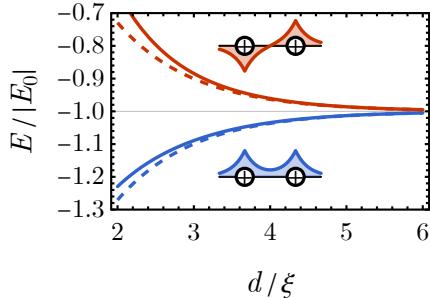
$$E_0 \begin{pmatrix} 1 & 2e^{-d/\xi} \\ 2e^{-d/\xi} & 1 \end{pmatrix} \begin{pmatrix} \psi_{\tilde{1}} \\ \psi_{\tilde{2}} \end{pmatrix} = E \begin{pmatrix} \psi_{\tilde{1}} \\ \psi_{\tilde{2}} \end{pmatrix}. \quad (63)$$

- Solving the eigen problem, one finds two eigen states $|\psi_{\pm}\rangle$ with the eigen energy E_{\pm}

$$E_{\pm} = E_0(1 \pm 2e^{-d/\xi}),$$

$$|\psi_{\pm}\rangle = \frac{1}{\sqrt{2}} (|\tilde{1}\rangle \pm |\tilde{2}\rangle) \propto |1\rangle \pm |2\rangle.$$

(64)



- Solid curve: exact energy.
- Dashed curve: approximate energy to the 1st order in $e^{-d/\xi}$ (given by the tight binding model).
- █: even parity, bonding orbital $|\psi_{+}\rangle$,
- █: odd parity, anti-bonding orbital $|\psi_{-}\rangle$

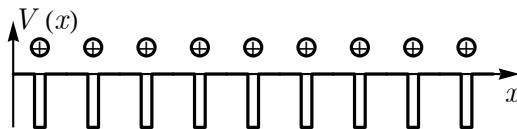
■ 1D Electronic Systems

■ Electron on 1D Lattice

A electron moving on the background of a lattice of positive ions.

$$H = -\frac{\hbar^2}{2m} \partial_x^2 + V(x) \quad (65)$$

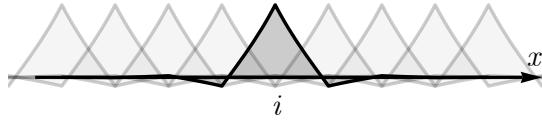
- **Periodic potential:** $V(x+a) = V(x)$, i.e. the potential is invariant under lattice translation $x \rightarrow x+a$.



Define a set of **tight binding basis**

$$\langle x|i\rangle = \psi_i(x) \propto e^{-|x-x_i|/\xi} + (\text{orthogonality corrections ...}), \quad (66)$$

where $x_i = ia$ is the position of the i th ion (i - **site index**, labels the lattice site).



- The lattice translation correspond to $|i\rangle \rightarrow |i+1\rangle$ for tight binding basis.

Expand the Hamiltonian H on the tight binding basis,

$$H = \sum_{ij} |i\rangle H_{ij} \langle j|, \quad (67)$$

where $H_{ij} \equiv \langle i| H |j\rangle$.

- The **lattice translation symmetry** implies

$$\langle i+1| H |j+1\rangle = \langle i| H |j\rangle, \quad (68)$$

i.e. H_{ij} only depends on the index *difference* $i - j$.

- Hermiticity** of the Hamiltonian requires

$$H_{ij} = H_{ji}^*. \quad (69)$$

- The Hamiltonian matrix must take the form of

$$H_{ij} = \begin{cases} -t_{i-j} & i > j \\ \epsilon_0 & i = j, \\ -t_{j-i}^* & i < j \end{cases} \quad (70)$$

or in the matrix form as

$$H = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots \\ \ddots & \epsilon_0 & -t_1^* & -t_2^* \\ \ddots & -t_1 & \epsilon_0 & -t_1^* \\ -t_2 & -t_1 & \epsilon_0 & \ddots \\ \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \quad (71)$$

- ϵ_0 - **on-site potential energy**.

- t_n - n th neighbor **hopping** parameter (kinetic energy). t_n is expected to decay exponentially

$$t_n \sim e^{-|x_n - x_0|/\xi} = e^{-n a / \xi}, \quad (72)$$

therefore t_n is often *truncated* to the first few leading ones (the few nearest neighbors hopping parameters).

■ Tight Binding Model and Energy Band

Truncate to 2nd nearest neighbor hopping. Assuming $t_1, t_2 \in \mathbb{R}$, the **tight binding Hamiltonian** reads

$$H = \epsilon_0 \sum_i |i\rangle \langle i| - t_1 \sum_i (|i+1\rangle \langle i| + \text{h.c.}) - t_2 \sum_i (|i+2\rangle \langle i| + \text{h.c.}), \quad (73)$$

where h.c. stands for the omitted term related by *Hermitian conjugation*.

Goal: solve the Schrödinger equation $H |\psi\rangle = E |\psi\rangle$, find the eigen states and the corresponding eigen energies of the electron.

It turns out that the Hamiltonian can be simply diagonalized by transforming to the **quasi-momentum basis** $|k\rangle$.

- The quasi-momentum basis and the tight binding basis are related Fourier / inverse Fourier transforms

$$|i\rangle = N^{-1/2} \sum_k e^{-i k x_i} |k\rangle,$$

$$|k\rangle = N^{-1/2} \sum_i e^{i k x_i} |i\rangle,$$

(74)

where N is the total number of sites in the lattice.

- Assuming N is even, \sum_k sums over

$$k = 0, \pm \frac{2\pi}{Na}, \dots, \pm \frac{2\pi m}{Na}, \dots, \pm \frac{2\pi(N/2-1)}{Na}, \frac{\pi}{a}.$$
(75)
- \sum_i sums over $i = 1, 2, \dots, N-1, N$.
- Substitute Eq. (74) into Eq. (73), the Hamiltonian is diagonalized

$$H = \sum_k \epsilon_k |k\rangle \langle k|,$$

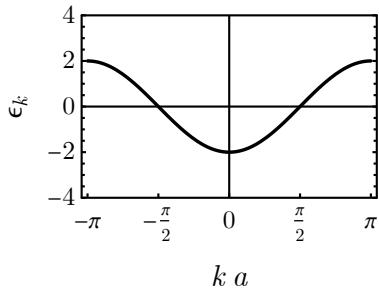
$$\epsilon_k = \epsilon_0 - 2 t_1 \cos(k a) - 2 t_2 \cos(2 k a).$$

(76)

Exc
4

Derive Eq. (76).

- **Dispersion relation** ϵ_k of the electron (also called **band structure**, **band dispersion**)



- The dispersion relation ϵ_k is *periodic* in the quasi-momentum, i.e.

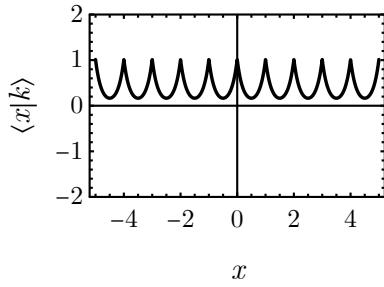
$$\epsilon_{k+\frac{2\pi}{a}} = \epsilon_k, \quad (79)$$

so the quasi-momentum k of electron can be taken to be in the **first Brillouin zone**
 $k \in (-\pi/a, \pi/a]$.

- **Energy band:** the allowed energy range of the electron. The electron can not take an energy outside the energy band (as there is no state outside the energy band for the electron to occupied).
- **Eigenstates** (quasi-momentum basis states) in real space representation

$$\begin{aligned}\langle x|k\rangle &= N^{-1/2} \sum_i e^{ikx_i} \langle x|i\rangle \\ &= N^{-1/2} \sum_i e^{ik a i} \psi_i(x).\end{aligned}\tag{80}$$

Tight binding basis ψ_i enveloped by a plane wave.

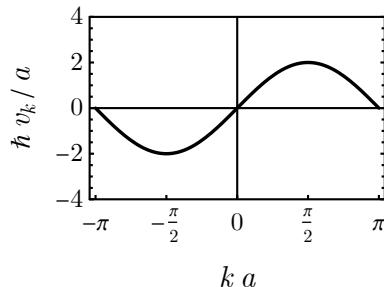


- **Group velocity** of the electron

$$v_k = \frac{1}{\hbar} \frac{\partial \epsilon_k}{\partial k}.\tag{81}$$

Take the dispersion relation ϵ_k in Eq. (76),

$$v_k = \frac{2 a t_1}{\hbar} \sin(k a) + \frac{4 a t_2}{\hbar} \sin(2 k a).\tag{82}$$



- The group velocity always *vanishes* ($v_k = 0$) at both the Brillouin zone *center* ($k = 0$) and zone *boundary* ($k = \pi/a$), because they are **inversion symmetric** points (i.e. $k \cong -k$) in the Brillouin zone. Since velocity is *odd* under inversion

$$v_{-k} = -v_k, \quad (83)$$

it must vanish at inversion symmetric momentum points.

- The quasi-momentum basis states $|k\rangle$ are **standing wave** states at $k = 0$ and $k = \pi/a$, i.e. the electron wave does not propagate and the group velocity vanishes. The standing wave at $k = \pi/a$ is caused by the strong back-scattering (Bragg scattering) of electron by the lattice.

- **Effective mass** m_{eff} of the electron

$$m_{\text{eff}}^{-1} = \frac{1}{\hbar} \frac{\partial v_k}{\partial k} = \frac{1}{\hbar^2} \frac{\partial^2 \epsilon_k}{\partial k^2}. \quad (84)$$

Take the dispersion relation ϵ_k in Eq. (76),

$$m_{\text{eff}}^{-1} = \frac{2 a^2 t_1}{\hbar^2} \cos(k a) + \frac{8 a^2 t_2}{\hbar^2} \cos(2 k a). \quad (85)$$

- At band *bottom* ($k = 0$), the effective mass is *positive*

$$m_{\text{eff}} = \frac{\hbar^2}{2 a^2(t_1 + 4 t_2)}. \quad (86)$$

- At band *top*, the effective mass is *negative*. For example, for $t_2 < t_1/4$, the band top is at $k = \pi/a$, where the effective mass is

$$m_{\text{eff}} = \frac{\hbar^2}{2 a^2(-t_1 + 4 t_2)}. \quad (87)$$

When the effective mass is negative, the electron velocity decreases with increasing momentum. The negative effective mass is a peculiar feature of electron on the lattice.

■ Thermodynamic Limit and Density of State

The total number N of lattice sites was introduced to regularize the Fourier transform. However, the physical results (intensive properties of the system) should have be well-defined in the **thermodynamic limit** $N \rightarrow \infty$.

In particular, the *momentum summation* can be replaced by a *momentum integration* in the thermodynamic limit $N \rightarrow \infty$, as the momentum grid spacing $2\pi/(N a) \rightarrow 0$,

$$\sum_k = N a \int_{-\pi}^{\pi} \frac{dk}{2\pi} = V \int_{-\pi}^{\pi} \frac{dk}{2\pi}, \quad (88)$$

where $V = N a$ is the (1D) volume of the system.

- *Extensive* property that involves summation \sum_k of states will be proportional to the volume V .
- *Intensive* property (extensive property per volume) eliminates the volume dependence, and has well-defined thermodynamic limit.

The *momentum integration* can be further converted to an *energy integration*,

$$\sum_k = V \int d\epsilon \sum_{\epsilon_k=\epsilon} \frac{1}{2\pi |\partial_k \epsilon_k|} = V \int d\epsilon \sum_{\epsilon_k=\epsilon} \frac{1}{2\pi \hbar |v_k|}. \quad (89)$$

Define the **density of state** $g(\epsilon)$ via

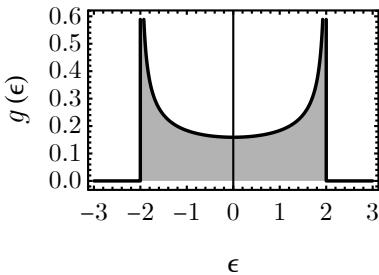
$$\sum_k = V \int d\epsilon g(\epsilon). \quad (90)$$

For 1D system,

$$g(\epsilon) = \sum_{\epsilon_k=\epsilon} \frac{1}{2\pi \hbar |v_k|}. \quad (91)$$

- For $\epsilon_k = -2t \cos(k a)$, we have $\hbar v_k = 2a t \sin(k a)$,

$$\begin{aligned} g(\epsilon) &= \sum_{-2t \cos(k a)=\epsilon} \frac{1}{4\pi a t |\sin(k a)|} \\ &= \frac{1}{2\pi a t |\sin(\arccos \frac{\epsilon}{2t})|} \\ &= \frac{1}{\pi a \sqrt{(2t)^2 - \epsilon^2}}. \end{aligned} \quad (92)$$



- The *divergences* of density of state near band edges are examples of **van Hove singularities**.
- The mid-band density of state saturates to $g(0) = 1/(2\pi a t)$.

**HW
1**

Consider adding a stagger potential u to the 1D tight binding model (assuming the nearest neighboring bond length to be 1, as the length unit)

$$H = -t \sum_i (|i+1\rangle\langle i| + \text{h.c.}) - u \sum_i (-1)^i |i\rangle\langle i|.$$

For $u \neq 0$, the primitive unit cell is enlarged from one site to two sites. The first Brillouin zone correspondingly shrinks to $[\pi/2, -\pi/2]$.

- (i) How many bands do you expect?
- (ii) Calculate the band dispersion for each band.

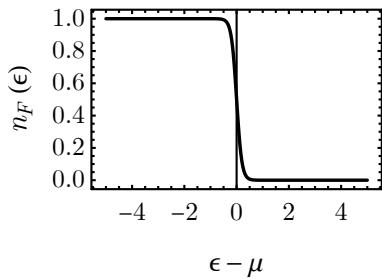
Solution (HW 1)

■ Fermi Statistics and Band Filling

By diagonalizing the electron Hamiltonian, we have just solved a **single-particle problem**, and obtained the eigenstates that an electron can occupy. When there is many electrons in the system, each eigenstate of the eigenenergy ϵ will have an **occupation probability** given by the **Fermi-Dirac distribution**

$$n_F(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}, \quad (96)$$

- $\beta = 1 / k_B T$, where T is the **temperature**.
- μ is the **chemical potential** (Fermi energy).



- The chemical potential is set by the **total number** N_e of electrons

$$N_e = 2 \sum_k n_F(\epsilon_k) = 2 \sum_k \frac{1}{e^{\beta(\epsilon_k-\mu)} + 1}. \quad (97)$$

The factor 2 in front of the summation takes into account the fact that each electron has *two* degenerated *spin* states.

- Then the **total internal energy** E of the electronic system is

$$E = 2 \sum_k \epsilon_k n_F(\epsilon_k) = 2 \sum_k \frac{\epsilon_k}{e^{\beta(\epsilon_k-\mu)} + 1}. \quad (98)$$

In the low-temperature ($T \rightarrow 0$) limit, electrons will simply occupy all states below the Fermi energy μ , such that Eq. (97) and Eq. (98) simplifies to

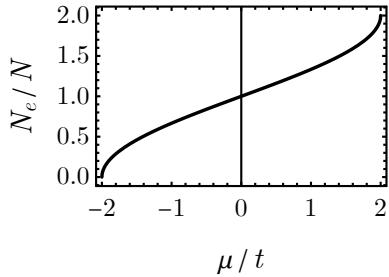
$$N_e = 2 \sum_{\epsilon_k < \mu} 1, \quad E = 2 \sum_{\epsilon_k < \mu} \epsilon_k. \quad (99)$$

- For $\epsilon_k = -2 t \cos(k a)$, use the density of state $g(\epsilon)$ in Eq. (92), the total number of electrons increases with μ from 0 to 2 as

$$N_e = 2 V \int_{-2t}^{\mu} d\epsilon g(\epsilon)$$

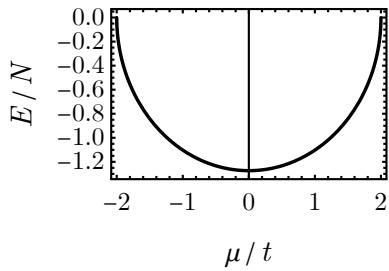
$$= \frac{2 V}{\pi a} \int_{-2t}^{\mu} d\epsilon \frac{1}{\sqrt{(2t)^2 - \epsilon^2}}$$

$$= \frac{2 N}{\pi} \left(\arcsin\left(\frac{\mu}{2t}\right) + \frac{\pi}{2} \right).$$



and the total internal energy varies with μ as

$$\begin{aligned} E &= 2 V \int_{-2t}^{\mu} d\epsilon \epsilon g(\epsilon) \\ &= \frac{2 V}{\pi a} \int_{-2t}^{\mu} d\epsilon \frac{\epsilon}{\sqrt{(2t)^2 - \epsilon^2}} \\ &= -\frac{2 N}{\pi} \sqrt{(2t)^2 - \mu^2}. \end{aligned} \tag{101}$$

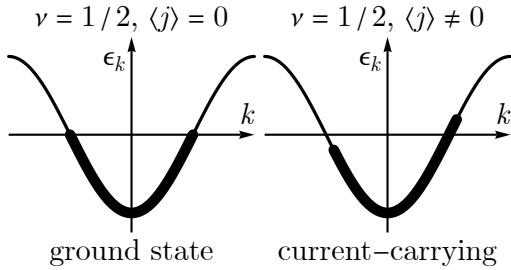


- **Filling fraction:** the fraction of a energy band filled by electrons

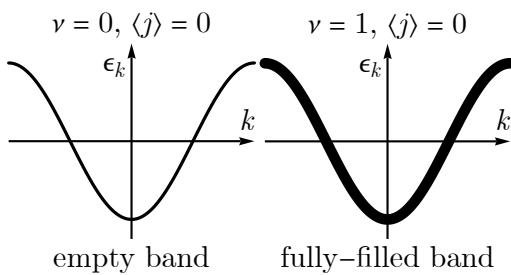
$$\nu = \frac{N_e}{2 N}, \tag{102}$$

where $2 N$ is the number of states (including 2-fold spin degeneracy) in the energy band. N is the number of sites in the lattice.

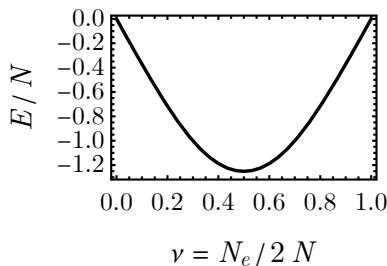
- When $0 < \nu < 1$, the many-body system of electrons forms a **metal** (in the non-interacting limit).



- In the **many-body ground state**: electrons occupy all states from the band bottom up to the designated filling fraction \Rightarrow total energy E is minimized.
- A *current-carrying* excited state can be created by an *imbalanced* occupation of electrons, such that there are more electrons on the $v_k > 0$ side than those on the $v_k < 0$ side. $\Rightarrow \langle j \rangle = e \sum_k \langle v_k \rangle \neq 0$. \Rightarrow Metal can conduct electricity.
- However, if the band is *empty* ($\nu = 0$) or *fully filled* ($\nu = 1$), the current-carrying state can not be constructed. \Rightarrow The system can not conduct electricity, hence an **insulator** (also called **band insulator**).



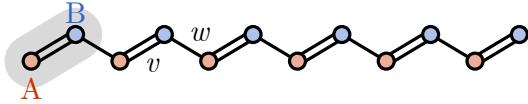
- **Metallic bond**: N atoms can gain energy jointly by allowing their electrons to delocalize and hybridize across the whole system. This energy gain binds all atoms together forming a metallic state.



- Given ϵ_k , one can calculate E v.s. N_e by tuning μ in Eq. (99).
- The total energy E is typically minimized at some $\nu \in (0, 1) \Rightarrow$ electrons forming a metallic state.

■ Su-Schrieffer-Heeger Model

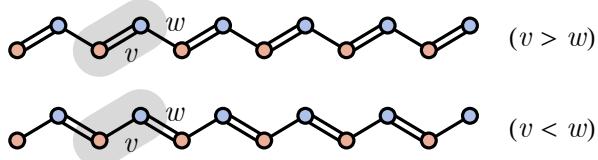
The Su-Schrieffer-Heeger (SSH) model is the simplest model of **symmetry protected topological** (SPT) state of electrons. It describes electrons in a poly-acetylene structure



- Each *unit cell* (gray shaded) now contains *two* atoms (labeled by *A* and *B*). Each lattice site is labeled jointly by the **unit cell index** *i* and the **sublattice label** *A / B*, such that a set of **tight binding basis** can be defined

$$\dots, |i,A\rangle, |i,B\rangle, |i+1,A\rangle, |i+1,B\rangle \dots \quad (103)$$

- The **hopping parameters** are different on the *double bond* and the *single bond* (double bond is shorter \Rightarrow larger hopping).
 - *v*: *intra-unit-cell hopping*,
 - *w*: *inter-unit-cell hopping*.



The **tight binding Hamiltonian**:

$$H = -v \sum_i (|i,B\rangle \langle i,A| + \text{h.c.}) - w \sum_i (|i+1,A\rangle \langle i,B| + \text{h.c.}) \quad (104)$$

Assuming *periodic boundary condition*, the system respect *lattice translation symmetry*, such that the *quasi-momentum* is a good quantum number. The Hamiltonian can be diagonalized by transforming to the **quasi-momentum basis** (defined separately on each sublattice)

$$\begin{aligned} |k,A\rangle &= N^{-1/2} \sum_i e^{i k x_i} |i,A\rangle, \\ |k,B\rangle &= N^{-1/2} \sum_i e^{i k x_i} |i,B\rangle, \end{aligned} \quad (105)$$

where $x_i = i$ (with unit cell size set to $a = 1$), and N is the number of unit cells on the lattice. The inverse transformation is given by

$$\begin{aligned} |i,A\rangle &= N^{-1/2} \sum_k e^{-i k x_i} |k,A\rangle, \\ |i,B\rangle &= N^{-1/2} \sum_k e^{-i k x_i} |k,B\rangle, \end{aligned} \quad (106)$$

where \sum_k sums over $k \in (-\pi, \pi]$ in the **first Brillouin zone** with momentum step size $2\pi/N$.

The Hamiltonian in Eq. (104) becomes

$$\boxed{H = \sum_k (f_k |k,B\rangle\langle k,A| + f_k^* |k,A\rangle\langle k,B|), \\ f_k = -v - w e^{ik}.} \quad (107)$$

Exc 5 Derive Eq. (107).

- Represent in the $\{|k,A\rangle, |k,B\rangle\}$ basis, H takes the matrix form

$$H \simeq \bigoplus_k H_k, \quad H_k \simeq \begin{pmatrix} 0 & f_k^* \\ f_k & 0 \end{pmatrix}, \quad (109)$$

No mixing between different momentum sectors \Rightarrow the Hamiltonian can be diagonalized in each momentum sector independently.

- Goal: find eigen vectors

$$|k,m\rangle = u_{k,m,A} |k,A\rangle + u_{k,m,B} |k,B\rangle \\ \simeq \begin{pmatrix} u_{k,m,A} \\ u_{k,m,B} \end{pmatrix}. \quad (110)$$

such that

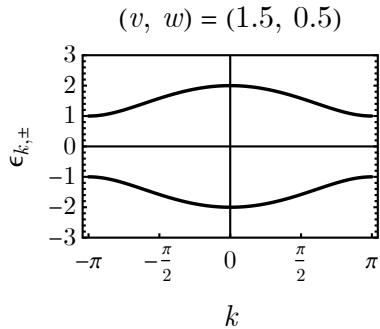
$$H_k |k,m\rangle = \epsilon_{k,m} |k,m\rangle, \quad (111)$$

or more explicitly

$$\begin{pmatrix} 0 & f_k^* \\ f_k & 0 \end{pmatrix} \begin{pmatrix} u_{k,m,A} \\ u_{k,m,B} \end{pmatrix} = \epsilon_{k,m} \begin{pmatrix} u_{k,m,A} \\ u_{k,m,B} \end{pmatrix}. \quad (112)$$

Eigen energies \Rightarrow band dispersion

$$\boxed{\epsilon_{k,\pm} = \pm |f_k| = \pm \sqrt{v^2 + w^2 + 2vw \cos k}} \quad (113)$$

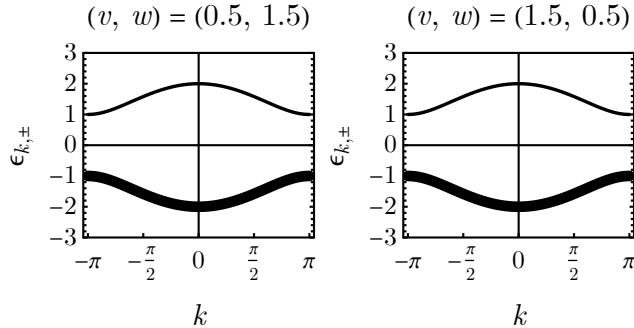


- There are *two* bands (labeled by \pm), matching the *number of sites* in the unit cell.
- **Band gap:** the range of energy between two bands. Electrons are forbidden to appear in the band gap (there is no state for the electron to occupy within the gap).

- Band gap opens at the *Brillouin zone boundary*, with the **gap size**

$$2\Delta = 2|v - w|. \quad (114)$$

- In the low-temperature ($T \rightarrow 0$) limit, electrons will fully occupy the lower band, forming a **band insulator**.



- The band structure does not distinguish $v > w$ from $v < w$, more information is contained in the *eigenstates*.

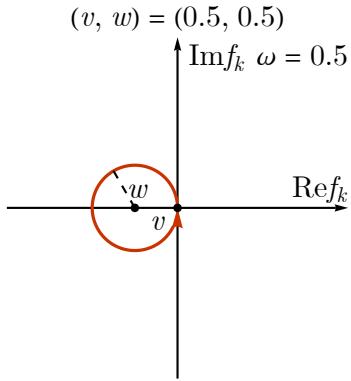
Eigenstates corresponding to $\epsilon_{k,\pm}$, represented as two-component state vectors in the $\{|k,A\rangle, |k,B\rangle\}$ basis

$$|k,\pm\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm f_k / |f_k| \end{pmatrix}. \quad (115)$$

- $f_k / |f_k| \in U(1) \cong S^1$ is a phase factor, that can wind around as $k \in S^1$ cycles over the first Brillouin zone.
- The map $f: S^1 \rightarrow S^1$ is classified by the **homotopy group** $\pi_1(S^1) \cong \mathbb{Z}$. Distinct homotopy classes are indexed by different **winding number**

$$\omega = \frac{1}{2\pi i} \int_{-\pi}^{\pi} dk \partial_k \ln f_k. \quad (116)$$

- $v > w$ (intra > inter): $\omega = 0$ (**trivial insulator**),
- $v < w$ (intra < inter): $\omega = 1$ (**topological insulator**).



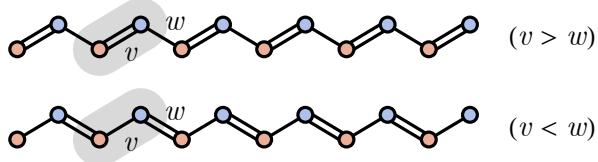
- A **topological phase transition** happens at $v = w$, where the system transition between the **trivial insulator** and the **topological insulator**, via gap closing and reopening.

More generally, the **winding number** can be defined for a **vector bundle** $|k,\pm\rangle$ over the Brillouin zone

$$\boxed{\begin{aligned} \omega_{\pm} &= \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \mathcal{A}_{k,\pm}, \\ \mathcal{A}_{k,\pm} &= -i \langle k,\pm | \partial_k | k,\pm \rangle, \end{aligned}} \quad (117)$$

- $\mathcal{A}_{k,\pm}$ is the **Berry connection** of the vector bundle,
- $2\pi\omega_{\pm}$ is the **Berry phase** accumulated along the Brillouin zone cycle, which is also called the **Zak phase** for the 1D case.

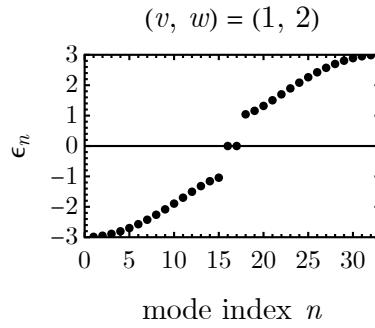
Topological edge mode. When $v < w$ (topological), there is a zero-energy dangling electron mode on each end of the chain (altogether two edge modes on both ends).



They can be observed in the spectrum. Put the tight binding Hamiltonian H Eq. (104) on an open chain (*open boundary condition*). The *lattice translation symmetry* is *broken* by the open ends, the *quasi-momentum* is no longer a good quantum number. One should diagonalize the Hamiltonian directly in tight binding basis Eq. (103)

$$H \simeq \begin{pmatrix} 0 & v & & & \\ v & 0 & w & & \\ & w & \ddots & \ddots & \\ & \ddots & \ddots & v & \\ & & v & 0 & \end{pmatrix}. \quad (118)$$

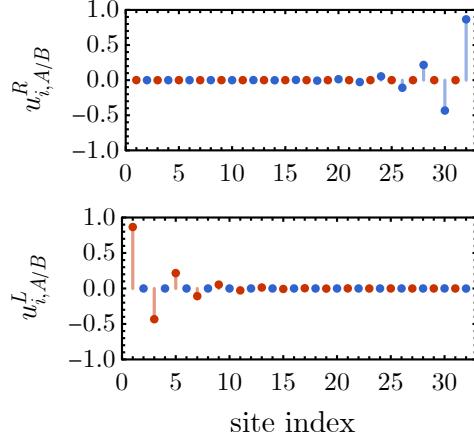
- Energy spectrum:



- When $v < w$ (topological), two zero-energy modes are left in the energy gap.
- Edge states (zero-energy model): assuming the states take the form of

$$|L/R\rangle = \sum_i (u_{i,A}^{L/R} |i,A\rangle + u_{i,B}^{L/R} |i,B\rangle). \quad (119)$$

The wave amplitude $u_{i,A/B}^\pm$ (■ on A sublattice, □ on B sublattice) are plotted for both zero modes:



- The wave amplitude decays exponentially from the edge with an localization length ξ , e.g.

$$|u_{i,A}^\pm| \sim e^{-x_i/\xi}. \quad (120)$$

Summary:

parameters	$v > w$	$v < w$
phase	trivial insulator	topological insulator
winding number	0	1
dimmerization	intra-unit-cell	inter-unit-cell
edge mode	no	yes (one / edge)
ground state deg.	1	2 (fix filling)

- HW 2**
- (i) Determine the edge mode localization length ξ as a function of hopping parameters v and w in the SSH model (assuming $w > v > 0$).
 - (ii) Show that near the critical point $v - w \rightarrow 0_-$, the localization length ξ is inversely proportional to the band gap $\Delta = |v - w|$.

Solution (HW 2)

■ Chiral Symmetry

Question: No matter how we tune v, w , the energy spectrum is always symmetric with respect to $E \rightarrow -E$, why?

- Sublattice projection operators

$$\begin{aligned} P_A &= \sum_i |i, A\rangle \langle i, A|, \\ P_B &= \sum_i |i, B\rangle \langle i, B|. \end{aligned} \quad (131)$$

- For any state $|\psi\rangle$ of an electron,
- $\langle\psi| P_A |\psi\rangle$ = probability to find the electron on sublattice A ,
- $\langle\psi| P_B |\psi\rangle$ = probability to find the electron on sublattice B .

- Chiral operator

$$S = P_A - P_B = \sum_i (|i, A\rangle \langle i, A| - |i, B\rangle \langle i, B|), \quad (132)$$

or, in the momentum space,

$$S = \sum_k (|k, A\rangle \langle k, A| - |k, B\rangle \langle k, B|), \quad (133)$$

Represent in the $\{|k, A\rangle, |k, B\rangle\}$ basis, S takes the matrix form

$$S \simeq \bigoplus_k S_k, \quad S_k \simeq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma^3. \quad (134)$$

- Under chiral transformation

$$\begin{cases} S |i, A\rangle = |i, A\rangle, \\ S |i, B\rangle = -|i, B\rangle. \end{cases} \quad \begin{cases} S_k |k, A\rangle = |k, A\rangle, \\ S_k |k, B\rangle = -|k, B\rangle. \end{cases} \quad (135)$$

B sublattice state gets a minus sign.

- The chiral transformation forms a \mathbb{Z}_2 group, as $S^2 = \mathbb{1}$ (where $\mathbb{1}$ stands for the identity operator).

- For any state $|\psi\rangle$ of an electron, $\langle\psi| S |\psi\rangle = \text{sublattice polarization}$.

Such that

$\langle\psi| S |\psi\rangle > 0$: more likely to find the electron on sublattice A ,

$\langle\psi| S |\psi\rangle < 0$: more likely to find the electron on sublattice B .

- **Chiral symmetry:** a unitary symmetry that anti-commutes with the Hamiltonian.

$$S H S = -H, \quad (136)$$

or, in the momentum space,

$$\forall k : S_k H_k S_k = -H_k. \quad (137)$$

Exc 6 Check Eq. (136) and Eq. (137).

Using the property $S^2 = \mathbb{1}$, Eq. (136) is equivalent to $S H = -H S$.

Spectral consequence of chiral symmetry: Let $|\psi_n\rangle$ be any eigenstate of H with eigen energy E_n , s.t.

$$H |\psi_n\rangle = E_n |\psi_n\rangle. \quad (140)$$

Chiral symmetry implies

$$H S |\psi_n\rangle = -S H |\psi_n\rangle = -S(E_n |\psi_n\rangle) = -E_n S |\psi_n\rangle, \quad (141)$$

meaning that $S |\psi_n\rangle$ is also an eigenstate of H but of an opposite eigen energy $-E_n$.

- If $E_n \neq 0$, $|\psi_n\rangle$ and $S |\psi_n\rangle$ are two distinct eigenstate of H with opposite eigen energies E_n and $-E_n \Rightarrow$ finite energy eigenstates always comes in $\pm E_n$ pairs.

- For example, in the momentum space, $H_k |k, \pm\rangle = \epsilon_{k,\pm} |k, \pm\rangle$, the eigen states indeed comes in pairs, related by the chiral transformation,

$$S_k |k, \pm\rangle = |k, \mp\rangle, \quad (142)$$

and the corresponding eigen energies are opposite to each other $\epsilon_{k,\pm} = \pm |f_k|$.

- However, even when the lattice translation symmetry is *broken* (e.g. on an open chain or in the presence of disorder) that quasi-momentum is not well-defined, the pairing of positive and negative energy states still holds through out the spectrum.

- If $E_n = 0$, $|\psi_n\rangle$ and $S |\psi_n\rangle$ are both zero-energy eigenstates of H , but they could be the same state. So there is no requirement for the zero energy states to come in pairs.

Sublattice polarization. The chiral symmetry $S H = -H S$ implies

$$\begin{aligned} \langle\psi_n| H S |\psi_n\rangle &= -\langle\psi_n| S H |\psi_n\rangle \\ &\Rightarrow E_n \langle\psi_n| S |\psi_n\rangle = -E_n \langle\psi_n| S |\psi_n\rangle \\ &\Rightarrow 2 E_n \langle\psi_n| S |\psi_n\rangle = 0. \end{aligned} \quad (143)$$

- If $E_n \neq 0$, then $\langle\psi_n| S |\psi_n\rangle = 0$, i.e. sublattice polarization should *vanish* for any finite energy eigenstate (the electron must appear on sublattice A and B with equal probability).

- This statement is manifest for momentum space eigenstates

$$|k, \pm\rangle = \frac{1}{\sqrt{2}} \left(|k, A\rangle \pm \frac{f_k}{|f_k|} |k, B\rangle \right). \quad (144)$$

- If $E_n = 0$, there is no restriction on $\langle \psi_n | S | \psi_n \rangle$. In fact, one can choose $|\psi_n\rangle$ to be the common eigenstate of S and H (as they commute in the zero-energy sector). Given that S only has two eigenvalues ± 1 , the zero-energy eigenstates can all be classified by

$$\langle \psi_n | S | \psi_n \rangle = \pm 1, \quad (145)$$

i.e. the electron in zero-energy state is either fully polarized to sublattice A or to sublattice B .

- The topological edge states are such examples.

■ Topological Phases of Band Insulators

Definition of topological phases for **band insulators**:

- (**No symmetry**)^{*} Two *band insulator* Hamiltonians H and H' are in the *same (invertible) topological phases*, if they can be *deformed* into each other without closing the *band gap*.

^{*} strictly speaking, band insulators already assumes the U(1) symmetry that corresponds to the *electron number conservation*. So “no symmetry” here means no additional symmetry apart from U(1).

- (**With symmetry**) Two *band insulator* Hamiltonians H and H' are in the *same symmetry protected topological (SPT) phases*, if they can be *deformed* into each other without closing the *band gap* and without breaking the *symmetry*.

Assuming lattice translation symmetry, the most general Hamiltonian for 1D electronic system with two-site unit cell takes the form of

$$H \simeq \bigoplus_k H_k, \quad H_k \simeq h_\mu(k) \sigma^\mu, \quad (146)$$

- As a 2×2 Hermitian matrix, H_k can always be decomposed to real combinations of Pauli matrices σ^μ

$$\sigma^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (147)$$

with the combination coefficients $h_\mu(k) \in \mathbb{R}$ ($\mu = 0, 1, 2, 3$).

- For example, the SSH model:

$$h_0(k) = 0, \quad h_1(k) = \text{Re } f_k, \quad h_2(k) = \text{Im } f_k, \quad h_3(k) = 0. \quad (148)$$

- Deforming H is to deform the $h_\mu(k)$ functions, subject to the periodic condition $h_\mu(k + 2\pi) = h_\mu(k)$ (i.e. $k \in S^1$).

The eigen energies of H_k is given by

$$\epsilon_{k,\pm} = h_0(k) \pm |\mathbf{h}(k)|, \quad (149)$$

where $\mathbf{h}(k) = (h_1(k), h_2(k), h_3(k))$ and $|\mathbf{h}(k)| = \sqrt{\mathbf{h}(k) \cdot \mathbf{h}(k)}$.

- **Gapping condition.** To maintain the band gap is to keep the vector $\mathbf{h}(k)$ finite length everywhere in the Brillouin zone

$$\forall k : |\mathbf{h}(k)| > 0. \quad (150)$$

or $\mathbf{h}(k) \in \mathbb{R}^3 \setminus \{\mathbf{0}\}$.

- Deformation *without symmetry*. All smooth deformations of the map $\mathbf{h} : S^1 \rightarrow \mathbb{R}^3 \setminus \{\mathbf{0}\}$ are classified by the homotopy group

$$\pi_1(\mathbb{R}^3 \setminus \{\mathbf{0}\}) \cong \pi_1(S^2) \cong 0, \quad (151)$$

which is a trivial group, meaning that all maps \mathbf{h} can be deformed into each other \Rightarrow Without additional symmetry (other than U(1)), all insulators in 1D are in the same phase (the trivial phase).

The **chiral symmetry** imposes additional constraints on the Hamiltonian.

$$\forall k : S_k H_k S_k = -H_k, \quad (152)$$

given $S_k = \sigma^3$, which requires

$$h_0(k) = h_3(k) = 0. \quad (153)$$

Exc 7 Derive Eq. (153) from Eq. (152), given Eq. (146).

In the presence of the chiral symmetry, $\mathbf{h}(k)$ is restricted to the h_1 - h_2 plane (excluding the origin), i.e. $\mathbf{h}(k) \in \mathbb{R}^2 \setminus \{\mathbf{0}\}$.

- Deformation under the *chiral symmetry*. All smooth deformation of the map $\mathbf{h} : S^1 \rightarrow \mathbb{R}^2 \setminus \{\mathbf{0}\}$ are classified by the homotopy group

$$\pi_1(\mathbb{R}^2 \setminus \{\mathbf{0}\}) \cong \pi_1(S^1) \cong \mathbb{Z}, \quad (157)$$

which is the integer addition group. Each class is labeled by an integer topological index ω , which corresponds to the winding number of \mathbf{h} around the origin in the h_1 - h_2 plane.

- *Protected by the chiral symmetry*, it is not possible to smoothly deform 1D insulators of different topological indices \Rightarrow topological insulators ($\omega \neq 0$) and the trivial insulator ($\omega = 0$) must be separated by gap-closing topological phase transitions.
- However, if the chiral symmetry is *broken*, the symmetry protection is lifted, and it becomes possible to smoothly deforming among all 1D insulators.

In the SSH model, the chiral symmetry can be broken by adding a **stagger potential** term u

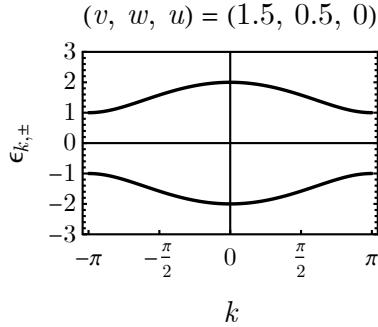
$$H = -v \sum_i (|i, B\rangle \langle i, A| + \text{h.c.}) - w \sum_i (|i+1, A\rangle \langle i, B| + \text{h.c.}) - u \sum_i (|i, A\rangle \langle i, A| - |i, B\rangle \langle i, B|). \quad (158)$$

Correspondingly, the momentum space Hamiltonian becomes

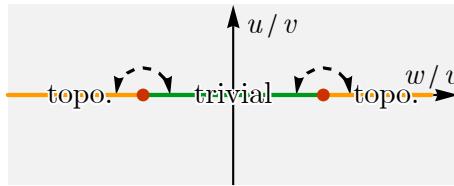
$$H \simeq \bigoplus_k H_k, H_k \simeq \begin{pmatrix} u & f_k^* \\ f_k & -u \end{pmatrix} = \operatorname{Re} f_k \sigma^1 + \operatorname{Im} f_k \sigma^2 + u \sigma^3, \quad (159)$$

- The **energy dispersion** becomes

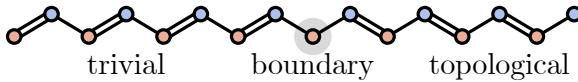
$$\epsilon_{k,\pm} = \pm \sqrt{|f_k|^2 + u^2} = \sqrt{v^2 + w^2 + 2 v w \cos k + u^2}. \quad (160)$$



- **Phase diagram.** With the chiral symmetry, $u = 0$, the trivial and topological phases must be separated by phase transitions. However, when the chiral symmetry is broken by $u \neq 0$, the topological transitions can be avoided / circumvented.



- Protected by the chiral symmetry, **topological edge mode** *must* exist on the *boundary* (the interface between trivial and topological states), otherwise one can proliferate the featureless boundary to avoid bulk transition (which contradict with the definition of SPT phases).



- **Interaction reduced classification.** The band homotopy classification indicates that 1D band insulators with charge conservation and chiral symmetries are \mathbb{Z} -classified. However, this is not the full story when interaction is taken into account. The stable classification is \mathbb{Z}_4 for 1D interacting fermionic SPT states in symmetry class AIII, meaning that the $\omega = 4$ insulator can be trivialized by interaction. [1]

[1] Lukasz Fidkowski, Alexei Kitaev. The effects of interactions on the topological classification of free fermion systems. arXiv:0904.2197.

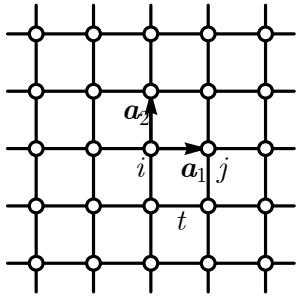
■ 2D Electronic Systems

■ Electron on Square Lattice

Consider an electron hopping on a 2D square lattice (as in cuprate superconductors).

$$\mathbf{x}_i = n_{i,1} \mathbf{a}_1 + n_{i,2} \mathbf{a}_2, \quad \begin{cases} \mathbf{a}_1 = (1, 0) \\ \mathbf{a}_2 = (0, 1) \end{cases}, \quad (161)$$

where $n_{i,1}, n_{i,2} \in \mathbb{Z}$.



- Define the nearest neighboring **bond vectors** (the vector that point from one site to its nearest neighboring site)

$$\begin{cases} \delta_1 = \mathbf{a}_1 = (1, 0) \\ \delta_2 = \mathbf{a}_2 = (0, 1) \\ \delta_3 = -\mathbf{a}_1 = (-1, 0) \\ \delta_4 = -\mathbf{a}_2 = (0, -1) \end{cases}. \quad (162)$$

Tight binding Hamiltonian (nearest neighbor hopping)

$$H = -t \sum_{\langle ij \rangle} (|i\rangle \langle j| + \text{h.c.}). \quad (163)$$

- i, j are site indices, which also label the tight binding basis $|i\rangle$.
- $\langle ij \rangle$ denotes i, j are adjacent on the lattice. $\sum_{\langle ij \rangle}$ sums over all such nearest neighbor links.

Switch to the **quasi-momentum basis**,

$$|\mathbf{k}\rangle = N^{-1/2} \sum_i e^{i \mathbf{k} \cdot \mathbf{x}_i} |i\rangle,$$

$$|i\rangle = N^{-1/2} \sum_{\mathbf{k}} e^{-i \mathbf{k} \cdot \mathbf{x}_i} |\mathbf{k}\rangle. \quad (164)$$

- $N = L_x \times L_y$ is the total number of unit cells (sites). L_x, L_y are the (linear) size of the lattice along x and y directions.
- $\sum_{\mathbf{k}}$ sums over momentum \mathbf{k} in the first Brillouin zone $(-\pi, \pi]^{\times 2}$ on a grid with spacings $2\pi/L_x$ and $2\pi/L_y$ along x and y directions.

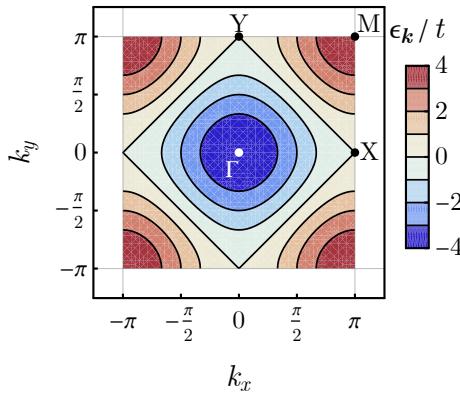
The Hamiltonian Eq. (163) is diagonalized in the quasi-momentum basis

$$\boxed{H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} |\mathbf{k}\rangle \langle \mathbf{k}|, \quad \epsilon_{\mathbf{k}} = -t \sum_a e^{i \mathbf{k} \cdot \delta_a} = -2t (\cos \mathbf{k} \cdot \mathbf{a}_1 + \cos \mathbf{k} \cdot \mathbf{a}_2).} \quad (165)$$

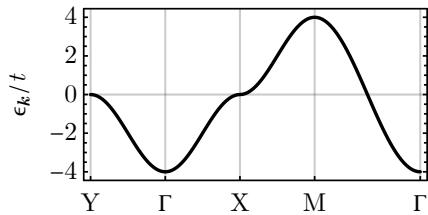
**Exc
8**

Derive Eq. (165).

Band dispersion $\epsilon_{\mathbf{k}}$ in the first Brillouin zone.



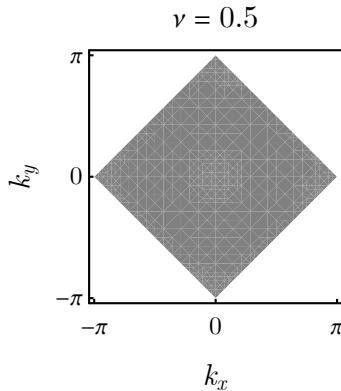
- High symmetry points of the Brillouin zone: $\Gamma(0, 0)$, $X(\pi, 0)$, $Y(0, \pi)$, $M(\pi, \pi)$.
- The band structure is often represented by plotting $\epsilon_{\mathbf{k}}$ along straight line segments connecting high symmetry points.



The electron will fill up the band up to the **Fermi surface**. Let ν be the **filling fraction**, and ϵ_F be the **Fermi energy**,

$$\nu = \frac{\sum_{k \in \text{BZ}} \Theta(\epsilon_F - \epsilon_k)}{\sum_{k \in \text{BZ}} 1}, \quad (169)$$

the filling fraction is the fraction that the Fermi sea takes up in the Brillouin zone.



- **Symmetry and the general shape of Fermi surface.** In the free space, electrons should have a *circular* Fermi surface, due to the SO(2) **rotation symmetry**. However, on a lattice, the full SO(2) rotation symmetry is *broken* to its *discrete subgroup*, such as \mathbb{Z}_4 for the square lattice. So the Fermi surface only have **four-fold symmetry** on a square lattice.
- **Small Fermi surface remains circular.** Because electrons are also *waves*, when the *wave length* is much larger than the *lattice spacing* (which is the case near the Γ point), the electron will not resolve the lattice structure (as the structure is below the *diffraction limit* of the electron wave), and will not experience the *symmetry breaking* effect caused by the lattice, hence the Fermi surface remains circular near the Γ point.
 - Expand the dispersion relation $\epsilon_{\mathbf{k}}$ in Eq. (165) around the Γ point ($\mathbf{k} \rightarrow 0$) (here the lattice constant $a = 1$ has been restored)

$$\begin{aligned}\epsilon_{\mathbf{k}} &= -4t + t a^2 \mathbf{k}^2 + O(k^4) \\ &= -4t + \frac{\hbar^2 \mathbf{k}^2}{2 m_{\text{eff}}} + O(k^4)\end{aligned}\tag{170}$$

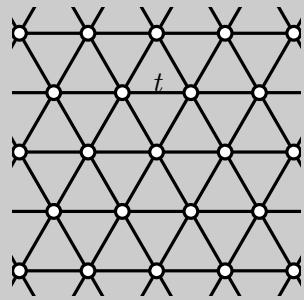
with the **effective mass** $m_{\text{eff}} = \hbar^2 / (2 t a^2)$ of the electron set by the hopping parameter t , similar to Eq. (86).

- **Large Fermi surface can be distorted.** As the Fermi surface approaches the *Brillouin zone boundary*, the lattice scattering effect gets more prominent, which distorts the Fermi surface to non-circular shape (such as the *square shape at half filling*).
- **“Broken” Fermi surface.** Beyond half filling, the Fermi surface can even touch the Brillouin zone boundary.
 - Note that whenever a Fermi surface touches the zone boundary, it must do so *perpendicularly*, because the normal component of the group velocity must be zero at the zone boundary.
 - The Fermi surface seems to be broken into segments, however, it is actually still continuous since the Brillouin zone is *periodic*.

- Electron v.s. hole Fermi surface. When the filling fraction approaches one, the Fermi surface looks circular again (if we look at the empty region). It can be viewed as filling *full band* with **holes**. Holes are **anti-particles** of electrons. High filling of electrons = low filling of holes \Rightarrow Fermi surface becomes circular as the hole filling is small.

HW
3

Consider a nearest neighbor hopping tight-binding model on a triangular lattice.

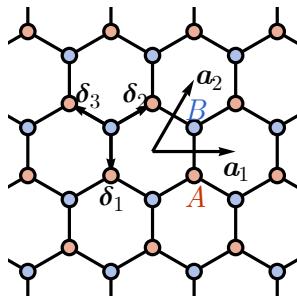


- (i) Calculate the band dispersion.
- (ii) Determine the effective mass at the band bottom.
- (iii) Determine the shape of the Fermi surface at the Fermi energy $\epsilon_F = 2 t$, and calculate the filling fraction to reach this Fermi energy.

Solution (HW 3)

■ Electron on Honeycomb Lattice

Consider an electron hopping on a 2D honeycomb lattice (as in graphene).



Each unit cell contains *two* sites. Define the *site* coordinates

$$\mathbf{x}_i = \mathbf{x}_{n,s} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + \mathbf{r}_s, \quad (176)$$

with $\mathbf{n} = (n_1, n_2) \in \mathbb{Z}^2$, $s = A, B$, and

$$\begin{cases} \mathbf{a}_1 = (\sqrt{3}, 0) \\ \mathbf{a}_2 = \left(\frac{\sqrt{3}}{2}, \frac{3}{2}\right) \end{cases}, \begin{cases} \mathbf{r}_A = (\sqrt{3}, 1) \\ \mathbf{r}_B = \left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right) \end{cases}. \quad (177)$$

- The site index $i \leftrightarrow (\mathbf{n}, s)$ contains the unit cell and sublattice labels jointly.
- Introduce the nearest neighboring displacement vectors for later convenience

$$\begin{cases} \boldsymbol{\delta}_1 = (0, -1) \\ \boldsymbol{\delta}_2 = \left(\frac{\sqrt{3}}{2}, \frac{1}{2} \right) \\ \boldsymbol{\delta}_3 = \left(-\frac{\sqrt{3}}{2}, \frac{1}{2} \right) \end{cases} . \quad (178)$$

Tight binding Hamiltonian (nearest neighbor hopping)

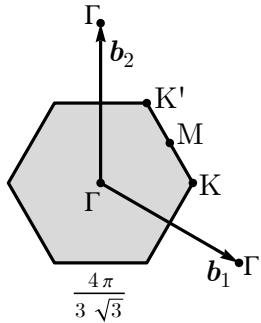
$$H = -t \sum_{\langle ij \rangle} (|i\rangle\langle j| + \text{h.c.}) \quad (179)$$

- The tight binding basis $|i\rangle$ is defined on each site, which may also be written as $|\mathbf{n}, s\rangle$ by the unit cell and sublattice labels.
- $\sum_{\langle ij \rangle}$ sums over nearest neighboring links $\langle ij \rangle$ on the honeycomb lattice.

Introduce the **quasi-momentum basis**, for each sublattice separately ($s = A, B$),

$$\begin{aligned} |\mathbf{k}, s\rangle &= N^{-1/2} \sum_n e^{i \mathbf{k} \cdot \mathbf{x}_i} |\mathbf{n}, s\rangle, \\ |\mathbf{n}, s\rangle &= N^{-1/2} \sum_k e^{-i \mathbf{k} \cdot \mathbf{x}_i} |\mathbf{k}, s\rangle. \end{aligned} \quad (180)$$

- N is the number of unit cells.
- The quasi-momentum is summed over the *first Brillouin zone*, which is a *hexagon* of side length $\frac{4\pi}{3\sqrt{3}}$.



- Recall that the first Brillouin zone is constructed as the *Wigner-Seitz cell* of the *reciprocal lattice*, spanned by the *reciprocal basis*

$$\begin{cases} \mathbf{b}_1 = \left(\frac{2\pi}{\sqrt{3}}, -\frac{2\pi}{3} \right) \\ \mathbf{b}_2 = \left(0, \frac{4\pi}{3} \right) \end{cases} . \quad (181)$$

- High symmetry points

$$\Gamma : (0, 0) + m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2,$$

$$K : \left(\frac{4\pi}{3\sqrt{3}}, 0 \right) + m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2,$$

$$K' : \left(-\frac{4\pi}{3\sqrt{3}}, 0 \right) + m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2,$$

$$M : \left(0, \frac{2\pi}{3} \right) + m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2.$$

For a tight binding Hamiltonian that respects the lattice translation symmetry, the transformation to the quasi-momentum basis is given by

$$\sum_{i,j} |i\rangle H_{ij} \langle j| = \sum_{\mathbf{k}} \sum_{s,s'} H_{\mathbf{k},ss'} |\mathbf{k},s\rangle \langle \mathbf{k},s'|,$$

$$H_{\mathbf{k},ss'} = \sum_n H_{ij} e^{i \mathbf{k} \cdot (\mathbf{x}_j - \mathbf{x}_i)} \text{ with } i = (\mathbf{0}, s), j = (\mathbf{n}, s').$$

(183)

Exc 9 Derive Eq. (183).

Apply Eq. (183) to the tight binding Hamiltonian Eq. (179),

$$H = \sum_{\mathbf{k}} (f_{\mathbf{k}} |\mathbf{k},B\rangle \langle \mathbf{k},A| + f_{\mathbf{k}}^* |\mathbf{k},A\rangle \langle \mathbf{k},B|),$$

$$f_{\mathbf{k}} = -t(e^{i \mathbf{k} \cdot \delta_1} + e^{i \mathbf{k} \cdot \delta_2} + e^{i \mathbf{k} \cdot \delta_3}).$$

(189)

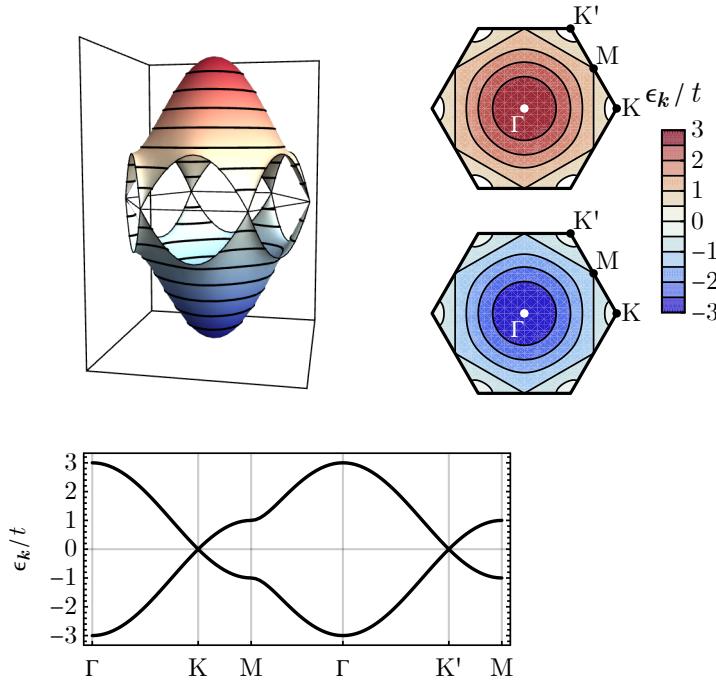
- Represent in the $\{|k,A\rangle, |k,B\rangle\}$ basis, H takes the matrix form

$$H \doteq \bigoplus_{\mathbf{k}} H_{\mathbf{k}}, H_{\mathbf{k}} \doteq \begin{pmatrix} 0 & f_{\mathbf{k}}^* \\ f_{\mathbf{k}} & 0 \end{pmatrix},$$
(190)

There are *two* bands (matching the number of sites in a unit cell). The **band dispersions** are given by the eigenvalues of $H_{\mathbf{k}}$

$$\epsilon_{\mathbf{k},\pm} = \pm |f_{\mathbf{k}}|.$$

(191)



- Two bands touch at the Brillouin zone corners (K and K' points).

Expand the Hamiltonian around the band touching points (to the leading order in the small momentum deviation κ)

$$\begin{aligned} H_{K+\kappa} &\simeq v_F \begin{pmatrix} 0 & \kappa_x - i\kappa_y \\ \kappa_x + i\kappa_y & 0 \end{pmatrix} + O(\kappa^2), \\ &= v_F (\kappa_x \sigma^1 + \kappa_y \sigma^2) + O(\kappa^2), \end{aligned} \quad (192)$$

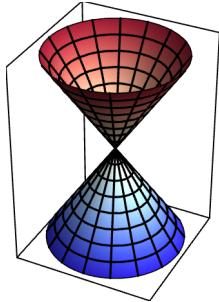
$$\begin{aligned} H_{K'+\kappa} &\simeq v_F \begin{pmatrix} 0 & -\kappa_x - i\kappa_y \\ -\kappa_x + i\kappa_y & 0 \end{pmatrix} + O(\kappa^2), \\ &= v_F (-\kappa_x \sigma^1 + \kappa_y \sigma^2) + O(\kappa^2), \end{aligned} \quad (193)$$

- These effective Hamiltonians describe 2D **Dirac fermions** of opposite chirality.
- When the chemical potential is set to the zero energy (at charge neutrality), the electronic system is in the **Dirac semi-metal** phase.
- **Dirac cones** (Dirac fermion dispersion). Near K and K' points, the energy is *linear* in the momentum deviation κ .

$$\epsilon_{K/K'+\kappa,\pm} = \pm v_F |\kappa|, \quad (194)$$

mimicking a *relativistic* particle with **Fermi velocity**

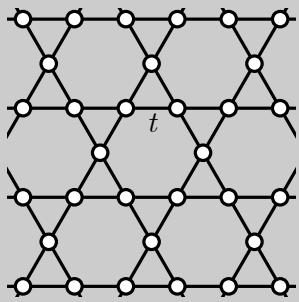
$$v_F = \frac{3}{2} t. \quad (195)$$



- The points K and K' are also called **Dirac points**, where the Dirac cones locate and the band gap close linearly. There are always *even* number of Dirac points in the Brillouin zone, known as the **Fermion doubling**.

Consider the nearest neighbor hopping tight binding model on a Kagome lattice (figure below).

HW
4



- How many bands do you expect?
- Write down the single-particle Hamiltonian in the momentum space.
- Diagonalize the Hamiltonian to calculate the band dispersions (you can use Mathematica), and show that there is an exact flat band.

Solution (HW 4)

■ Haldane Model

Adding *next nearest neighbor* hopping term λ (**Haldane hopping**), with purely *imaginary* amplitude,

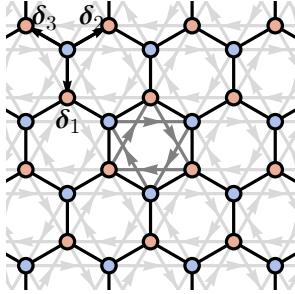
$$H = -t \sum_{\langle ij \rangle} (|i\rangle\langle j| + \text{h.c.}) + \lambda \sum_{\langle\langle ij \rangle\rangle} (i|i\rangle\langle j| + \text{h.c.}). \quad (201)$$

- Unlike real hopping, *imaginary* hopping is *directional*, as

$$(i|i\rangle\langle j|)^\dagger = -i|j\rangle\langle i|. \quad (202)$$

Rule: the electron hopping from j to i (i.e. the $|i\rangle\langle j|$ term) has a hopping coefficient $+i$ if j to i is along the *bond direction*.

- The bond directions are assigned in the following pattern



Transform to the quasi-momentum basis specified in Eq. (180), the Hamiltonian reads

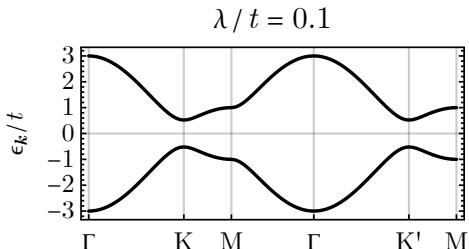
$$\boxed{H = \sum_{\mathbf{k}} (f_{\mathbf{k}} |\mathbf{k}, B\rangle \langle \mathbf{k}, A| + f_{\mathbf{k}}^* |\mathbf{k}, A\rangle \langle \mathbf{k}, B| + g_{\mathbf{k}} |\mathbf{k}, A\rangle \langle \mathbf{k}, A| - g_{\mathbf{k}} |\mathbf{k}, B\rangle \langle \mathbf{k}, B|), \\ f_{\mathbf{k}} = -t(e^{i\mathbf{k}\cdot\delta_1} + e^{i\mathbf{k}\cdot\delta_2} + e^{i\mathbf{k}\cdot\delta_3}), \\ g_{\mathbf{k}} = -2\lambda(\sin \mathbf{k} \cdot (\delta_1 - \delta_2) + \sin \mathbf{k} \cdot (\delta_2 - \delta_3) + \sin \mathbf{k} \cdot (\delta_3 - \delta_1)).} \quad (203)$$

- Represent in the $\{|\mathbf{k}, A\rangle, |\mathbf{k}, B\rangle\}$ basis, H takes the matrix form

$$H \simeq \bigoplus_{\mathbf{k}} H_{\mathbf{k}}, \quad H_{\mathbf{k}} \simeq \begin{pmatrix} g_{\mathbf{k}} & f_{\mathbf{k}}^* \\ f_{\mathbf{k}} & -g_{\mathbf{k}} \end{pmatrix}, \quad (204)$$

- The **band dispersions** are modified to

$$\epsilon_{\mathbf{k},\pm} = \pm \sqrt{|f_{\mathbf{k}}|^2 + g_{\mathbf{k}}^2}. \quad (205)$$



- The Haldane hopping term λ opens a **gap** between the two bands, gapping out Dirac fermions at K and K' .

Expand the Hamiltonian around Dirac points K and K'

$$\begin{aligned} H_{K+\kappa} &\simeq \begin{pmatrix} m v_F^2 & v_F(\kappa_x - i\kappa_y) \\ v_F(\kappa_x + i\kappa_y) & -m v_F^2 \end{pmatrix} + O(\kappa^2), \\ &= v_F(\kappa_x \sigma^1 + \kappa_y \sigma^2) + m v_F^2 \sigma^3 + O(\kappa^2), \end{aligned} \quad (206)$$

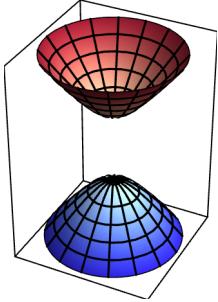
$$\begin{aligned} H_{K'+\kappa} &= \begin{pmatrix} -m v_F^2 & v_F(-\kappa_x - i \kappa_y) \\ v_F(-\kappa_x + i \kappa_y) & m v_F^2 \end{pmatrix} + O(\kappa^2), \\ &= v_F(-\kappa_x \sigma^1 + \kappa_y \sigma^2) - m v_F^2 \sigma^3 + O(\kappa^2), \end{aligned} \quad (207)$$

with the **Fermi velocity** v_F and the **Dirac mass** m given by

$$v_F = \frac{3t}{2}, \quad m = \frac{3\sqrt{3}\lambda}{v_F^2}. \quad (208)$$

The dispersion relation takes the form of a *massive* relativistic particle near Dirac points

$$\epsilon_{K/K'+\kappa,\pm} = \pm \sqrt{v_F^2 \kappa^2 + m^2 v_F^4}. \quad (209)$$



- When δk is small, the energy expands to

$$\epsilon_{K/K'+\kappa,\pm} = \pm \left(m v_F^2 + \frac{\kappa^2}{2m} + \dots \right), \quad (210)$$

which justifies the parameter m as the mass of the Dirac fermion (also the effective mass of electron/hole near the band edge).

- Even if starting from *non-relativistic* electrons in graphene, *relativistic* behaviors can **emerge** at low-energy. This provides opportunities to simulate certain aspects of fundamental particle physics in condensed matter systems.

■ Chern Insulator and Integer Quantum Hall Effect

The band gap closes and reopens as u goes across $\lambda = 0$, signifying a phase transition between two insulators. Is there any difference between the $\lambda > 0$ insulator and the $\lambda < 0$ insulator?

Band structure does not tell the difference, need to look at wave functions (eigen states). Let $|\mathbf{k}, \pm\rangle$ be the eigen states of H_k with eigen energies $\epsilon_{\mathbf{k}, \pm}$, i.e.

$$H_k |\mathbf{k}, \pm\rangle = \epsilon_{\mathbf{k}, \pm} |\mathbf{k}, \pm\rangle. \quad (211)$$

- **Berry connection** of the vector bundle $|\mathbf{k}, \pm\rangle$, like a *gauge potential* in the momentum space,

$$\mathcal{A}_{\mathbf{k}, \pm} = -i \langle \mathbf{k}, \pm | \nabla_{\mathbf{k}} | \mathbf{k}, \pm \rangle. \quad (212)$$

At each momentum point \mathbf{k} , the Berry connection has two components

$$\begin{aligned}\mathcal{A}_{\mathbf{k},\pm}^x &= -i \langle \mathbf{k}, \pm | \partial_{k_x} | \mathbf{k}, \pm \rangle, \\ \mathcal{A}_{\mathbf{k},\pm}^y &= -i \langle \mathbf{k}, \pm | \partial_{k_y} | \mathbf{k}, \pm \rangle.\end{aligned}\quad (213)$$

- **Berry curvature:** *curl of Berry connection* (taking the z component), like a *magnetic field* in the momentum space,

$$\mathcal{F}_{\mathbf{k},\pm} = \hat{z} \cdot (\nabla_{\mathbf{k}} \times \mathcal{A}_{\mathbf{k},\pm}),$$

(214)

or in term of components

$$\mathcal{F}_{\mathbf{k},\pm} = \partial_{k_x} \mathcal{A}_{\mathbf{k},\pm}^y - \partial_{k_y} \mathcal{A}_{\mathbf{k},\pm}^x. \quad (215)$$

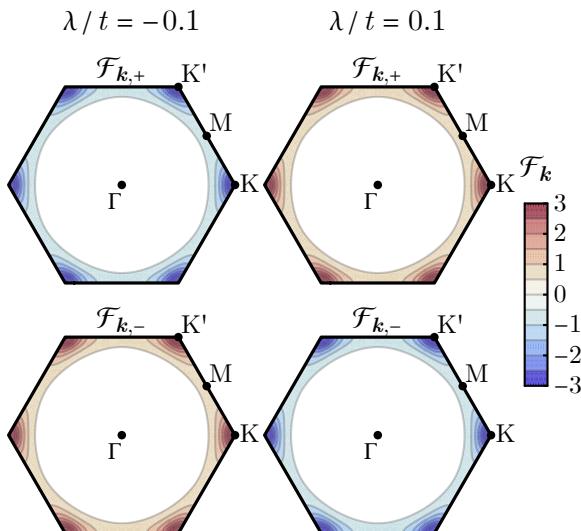
- For 2×2 Hamiltonian of the form $H_{\mathbf{k}} \simeq \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma}$, the Berry curvature is given by

$$\mathcal{F}_{\mathbf{k},\pm} = \pm \frac{1}{2 |\mathbf{h}(\mathbf{k})|^3} \mathbf{h}(\mathbf{k}) \cdot (\partial_{k_x} \mathbf{h}(\mathbf{k}) \times \partial_{k_y} \mathbf{h}(\mathbf{k})). \quad (216)$$

**Exc
10**

Prove Eq. (216).

- Apply Eq. (216) to the Haldane model, one can show the distribution of Berry curvature in the Brillouin zone (for both upper and lower bands) as a function of λ



- What is the physical effect of magnetic field in the momentum space? Recall: magnetic field \mathbf{B} in the real space \rightarrow electron will experience a Lorentz force

$$\frac{d\mathbf{k}}{dt} \propto -\mathbf{v} \times \mathbf{B} = -\frac{d\mathbf{x}}{dt} \times \mathbf{B}. \quad (227)$$

By analogy, switching from real space to momentum space effectively exchanges coordinate and momentum,

$$\frac{d\mathbf{x}}{dt} = -\frac{d\mathbf{k}}{dt} \times \mathcal{F}. \quad (228)$$

In the presence of an external electric field \mathbf{E}

$$\frac{\hbar d\mathbf{k}}{dt} = -e \mathbf{E}, \quad (229)$$

this will contribute to the current \mathbf{J} by

$$\mathbf{J} = -e \frac{d\mathbf{x}}{dt} = \frac{e^2}{\hbar} \mathcal{F} \times \mathbf{E}. \quad (230)$$

So $(e^2 / \hbar) \mathcal{F}_{k,\alpha}$ is the contribution to the Hall conductance from a single state .

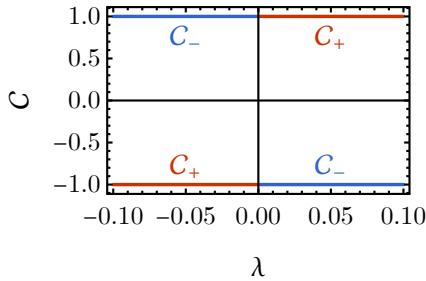
- **Chern number:** integration of *Berry curvature* over the *first Brillouin zone* (in unit of 2π), like the total *magnetic flux* through the Brillouin zone,

$$C_{\pm} = \frac{1}{2\pi} \int_{\text{BZ}} d^2\mathbf{k} \mathcal{F}_{k,\pm}. \quad (231)$$

- The Chern number C_{\pm} is separately define for each band (labeled by \pm). For two-band system, Chern numbers are opposite between upper and lower bands, $C_+ = -C_-$.
- It turns out that $C_{\pm} \in \mathbb{Z}$ is always an integer. For Haldane model,

$$C_{\pm} = \pm \operatorname{sgn} \lambda. \quad (232)$$

- As λ is tuned across $\lambda = 0$, the Chern number exchanges between the upper and lower bands.



- The Chern number is a *topological number* of the vector bundle $|\mathbf{k}, \pm\rangle$. The 2D insulators with non-trivial Chern numbers in *occupied bands* are called **Chern insulators**. The jump of Chern number at $\lambda = 0$ signifies a **topological transition** between two distinct Chern insulators.
- The **Hall conductance** of the Chern insulator (at the low-temperature limit) equals the total the Chern numbers C_{α} of all occupied bands (bands below the Fermi level) times the quantum conductance e^2 / h .

$$\sigma_H = \frac{e^2}{h} \sum_{\alpha \in \text{occ.}} C_{\alpha}. \quad (233)$$

Argument: the Hall conductance of a band averages the contribution from all states in the band

$$\sigma_H = \frac{e^2}{\hbar} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \mathcal{F}_{\mathbf{k},\alpha} = \frac{e^2}{\hbar} \frac{1}{2\pi} \int d^2 \mathbf{k} \mathcal{F}_{\mathbf{k},\alpha} = \frac{e^2}{\hbar} C_\alpha. \quad (234)$$

- The phenomenon that the Hall conductance *quantize* to *integer* multiples of e^2 / h is called the **integer quantum Hall effect**.

Near the phase transition, the Berry curvature concentrated at the Dirac points. Around each Dirac point, the effective Hamiltonian reads (setting $v_F = 1$ for simplicity)

$$\begin{aligned} H_{K+\kappa} &\simeq \kappa_x \sigma^1 + \kappa_y \sigma^2 + m \sigma^3, \\ H_{K'+\kappa} &\simeq -\kappa_x \sigma^1 + \kappa_y \sigma^2 - m \sigma^3, \end{aligned} \quad (235)$$

- Using Eq. (216), the Berry curvature can be evaluated

$$\mathcal{F}_{K+\kappa,\pm} = \mathcal{F}_{K'+\kappa,\pm} = \pm \frac{m}{2(\kappa^2 + m^2)^{3/2}} \quad (236)$$

- Each *massive Dirac fermion* contribute $\pm 1/2$ to the band Chern number. For example, around K point

$$C_{K,\pm} = \frac{1}{2\pi} \int d^2 \kappa \mathcal{F}_{K+\kappa,\pm} = \pm \frac{1}{2} \frac{m}{|m|} = \pm \frac{1}{2} \operatorname{sgn} m. \quad (237)$$

Same result will be obtained around K' , $C_{K,\pm} = C_{K',\pm} = \pm \frac{1}{2} \operatorname{sgn} m$, such that the Chern number follows

$$C_\pm = C_{K,\pm} + C_{K',\pm} = \pm \operatorname{sgn} m, \quad (238)$$

confirming the observation in Eq. (232).

■ Classifying Topological Insulators in 2D

Two band insulators can belong to the same or different topological phases, depending on whether or not there exist a *smooth deformation* of the Hamiltonian that connects the two insulators *without closing the gap*.

Assuming translation symmetry, any 2D band insulator can be described by an effective Hamiltonian that focus on the upper and lower bands across the Fermi level

$$H \simeq \bigoplus_k H_k, \quad H_k \simeq \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma}. \quad (239)$$

- The **band gap** is set by $|\mathbf{h}(\mathbf{k})|$. To keep the gap open, must have

$$\forall \mathbf{k} : |\mathbf{h}(\mathbf{k})| > 0, \quad (240)$$

meaning that $\mathbf{h}(\mathbf{k}) \in \mathbb{R}^3 \setminus \{\mathbf{0}\}$. For 2D system, $\mathbf{k} \in T^2$ (2D torus).

- All smooth deformations of the function $\mathbf{h} : T^2 \rightarrow \mathbb{R}^3 \setminus \{\mathbf{0}\}$ are classified by the homotopy group

$$\pi_2(\mathbb{R}^3 \setminus \{\mathbf{0}\}) \cong \pi_2(S^2) \cong \mathbb{Z}, \quad (241)$$

which is the integer addition group. Each class is labeled by an integer topological index ω , which corresponds to the winding number of \mathbf{h} in the 2D Brillouin zone

$$\omega = \frac{1}{4\pi} \int_{\text{BZ}} d^2 k \frac{1}{|\mathbf{h}(\mathbf{k})|^3} \mathbf{h}(\mathbf{k}) \cdot (\partial_{k_x} \mathbf{h}(\mathbf{k}) \times \partial_{k_y} \mathbf{h}(\mathbf{k})). \quad (242)$$

- By Eq. (216), the winding number is the same as the **Chern number**. Thus topological insulators (with no additional symmetry other than U(1)) is classified by the band Chern number.

Both $\lambda > 0$ and $\lambda < 0$ insulators are *non-trivial* topological insulators with Chern number ∓ 1 in the lower band. The trivial insulator in this system can be achieved by adding a **staggered on-site potential** δ

$$H = -t \sum_{\langle ij \rangle} (|i\rangle \langle j| + \text{h.c.}) + \lambda \sum_{\langle\langle ij \rangle\rangle} (i |i\rangle \langle j| + \text{h.c.}) + \delta \sum_i (-)^i |i\rangle \langle i|, \quad (243)$$

where $(-)^i = +1$ if $i \in A$ and $(-)^i = -1$ if $i \in B$.

- In the momentum space, the Hamiltonian still takes the form of

$$H \simeq \bigoplus_{\mathbf{k}} H_{\mathbf{k}}, \quad H_{\mathbf{k}} \simeq \begin{pmatrix} g_{\mathbf{k}} & f_{\mathbf{k}}^* \\ f_{\mathbf{k}} & -g_{\mathbf{k}} \end{pmatrix}, \quad (244)$$

but the function $g_{\mathbf{k}}$ is updated to

$$g_{\mathbf{k}} = \delta - 2\lambda (\sin k_x (\delta_1 - \delta_2) + \sin k_y (\delta_2 - \delta_3) + \sin k_z (\delta_3 - \delta_1)). \quad (245)$$

- Expanding around K and K' ,

$$\begin{aligned} H_{K+\kappa} &\simeq v_F (\kappa_x \sigma^1 + \kappa_y \sigma^2) + m_K v_F^2 \sigma^3 + O(\kappa^2), \\ H_{K'+\kappa} &\simeq v_F (-\kappa_x \sigma^1 + \kappa_y \sigma^2) - m_{K'} v_F^2 \sigma^3 + O(\kappa^2), \end{aligned} \quad (246)$$

the Dirac masses are different

$$\begin{aligned} m_K &= \frac{1}{v_F^2} (3 \sqrt{3} \lambda + \delta), \\ m_{K'} &= \frac{1}{v_F^2} (3 \sqrt{3} \lambda - \delta). \end{aligned} \quad (247)$$

- The band Chern numbers

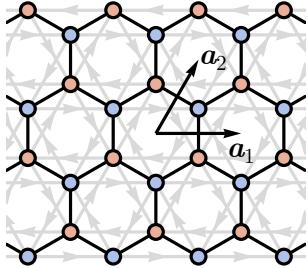
$$C_{\pm} = C_{K,\pm} + C_{K',\pm} = \pm \frac{1}{2} (\text{sgn } m_K + \text{sgn } m_{K'}). \quad (248)$$

If $\lambda = 0$ and $\delta \neq 0$, the masses are *opposite* between K and K' valleys \Rightarrow the Chern number from both valleys *cancels*, i.e. $C_{\pm} = 0 \Rightarrow$ the insulator is in the **trivial** phase.

■ Chiral Edge Mode

A prominent feature of the *Chern insulators* lies in the robust *chiral edge modes*. Consider placing the Haldane model on a honeycomb lattice with

- *periodic* boundary condition along x -direction (preserving translation symmetry along x -direction, k_x is still well-defined),
- *open* boundary condition along y -direction (top and bottom edges breaks translation symmetry along y -direction, can not define k_y),



Use mixed basis (transform to the momentum space only in the x -direction)

$$|k_x, y_i, s\rangle = \sum_{x_i} e^{-i k_x x_i} |i\rangle. \quad (249)$$

- The Hamiltonian is diagonal in k_x (because k_x is a good quantum number)

$$H = \sum_{k_x} |k_x\rangle H(k_x) \langle k_x|, \quad (250)$$

where

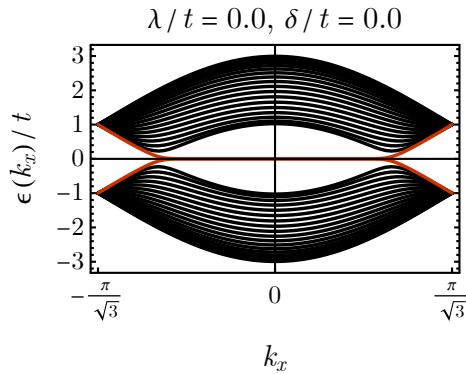
$$\begin{aligned} H(k_x) &= H_t(k_x) + H_\lambda(k_x) + H_\delta(k_x) \\ H_t(k_x) &= -t \sum_y \left(|y, B\rangle \langle y, A| + 2 \cos \frac{\sqrt{3} k_x}{2} |y+a_y, A\rangle \langle y, B| + \text{h.c.} \right) \\ H_\lambda(k_x) &= -2\lambda \sum_{k_x, y} \left(\sin \sqrt{3} k_x (|y, A\rangle \langle y, A| - |y, B\rangle \langle y, B|) - \right. \\ &\quad \left. \sin \frac{\sqrt{3} k_x}{2} (|y+a_y, A\rangle \langle y, A| - |y+a_y, B\rangle \langle y, B| + \text{h.c.}) \right) \\ H_\delta &= \delta \sum_{k_x, y} (|y, A\rangle \langle y, A| - |y, B\rangle \langle y, B|), \end{aligned} \quad (251)$$

with $a_y = 3/2$ being the inter-layer spacing.

- Further diagonalize $H(k_x)$ for every k_x

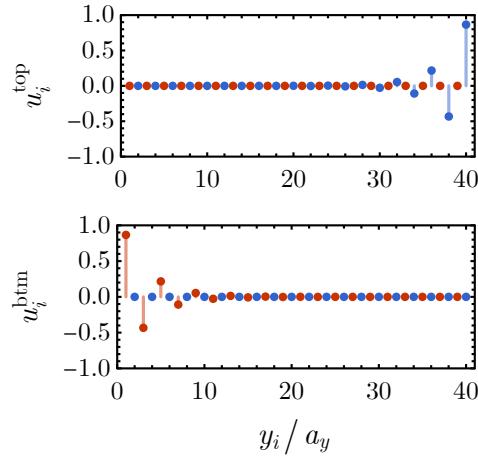
$$H(k_x) |u_n(k_x)\rangle = \epsilon_n(k_x) |u_n(k_x)\rangle \quad (252)$$

Bulk modes (in black) and **edge modes** (in red)



- Edge mode wave function (y -dependence). Edge modes are confined on the boundary. The wave functions decay exponentially into the bulk.

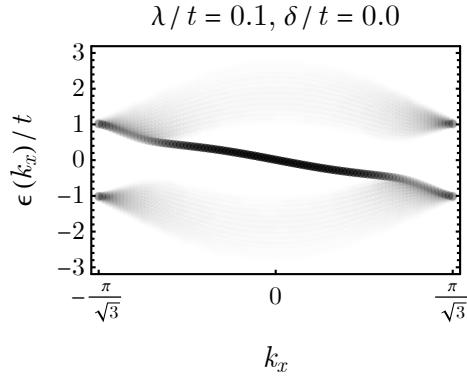
$$k_x = 0.0$$



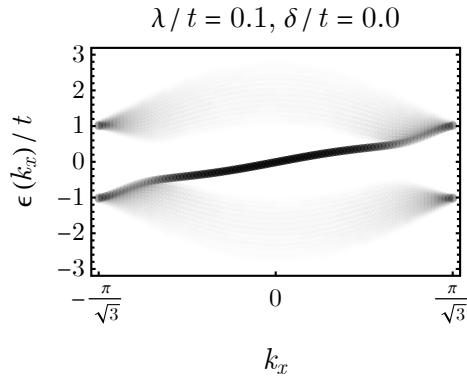
- Color every point $(k_x, \epsilon_n(k_x))$ by the weight of the corresponding mode $|u_n(k_x)\rangle$ on a given site. Define the **spectral function** $A_{y,s}$ on layer y sublattice s ,

$$A_{y,s}(k_x, \epsilon) = \sum_n |\langle y,s | u_n(k_x) \rangle|^2 \delta(\epsilon - \epsilon_n(k_x)). \quad (253)$$

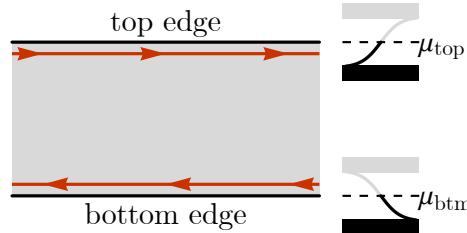
- **Bottom boundary** ($y = 1, s = A$)



- Effective dispersion of boundary modes: $\epsilon(k_x) \simeq -v k_x \Rightarrow$ **Left-moving** modes.
- Edge modes merge into bulk modes as the dispersion touches the bulk band.
- **Top boundary** ($y = L_y, s = B$)

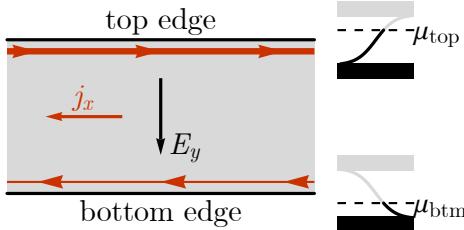


- Effective dispersion of boundary modes: $\epsilon(k_x) \simeq +v k_x \Rightarrow$ **Right-moving** modes.
- Edge modes merge into bulk modes as the dispersion touches the bulk band.
- **Chiral edge mode:** The edge mode circulates around the material in a chiral manner.



- **Quantized Hall conductance.** An electric field E_y creates electrostatic potential difference V_y between top and bottom boundaries \Rightarrow difference in electron chemical potentials μ_{top} and μ_{btm}

$$-e E_y L_y = -e V_y = \mu_{\text{top}} - \mu_{\text{btm}}, \quad (254)$$



more electrons occupy the top edge modes compared to bottom edge modes

$$N_{\text{top}} - N_{\text{btm}} = \frac{k_{x,\text{top}} - k_{x,\text{btm}}}{(2\pi/L_x)} = \frac{\mu_{\text{top}} - \mu_{\text{btm}}}{v\hbar(2\pi/L_x)} = \frac{-eE_yL_xL_y}{v\hbar}, \quad (255)$$

more right-moving electrons than left-moving electrons contributes to a net current

$$I_x = j_x L_y = -e v \frac{N_{\text{top}} - N_{\text{btm}}}{L_x} = \frac{e^2 E_y L_y}{h}. \quad (256)$$

Hall conductance σ_H is defined by

$$j_x = \sigma_H E_y, \quad (257)$$

Eq. (256) implies

$$\sigma_H = \frac{e^2}{h}. \quad (258)$$

which is indeed quantized (integer) in unit of the quantum conductance e^2/h .

- **Bulk-boundary correspondence.** The number of chiral edge modes (boundary property) \Leftrightarrow the quantized Hall conductance / the band Chern number (bulk property).

■ General Theory of Electrons in Crystals

■ Nearly Free Electron Model

The **tight binding models** provides a **real-space** perspective to understand electrons in a crystal. An alternative approach is the **nearly free electron model**, which provides a **momentum-space** perspective to the same problem.

Start with *free electron* in the empty space, the Hamiltonian is *diagonal* in *momentum* eigen basis

$$H_0 = \sum_k |\mathbf{k}\rangle \frac{\hbar^2 k^2}{2m} \langle \mathbf{k}|. \quad (259)$$

- $|\mathbf{k}\rangle$: plane wave state of electron $\psi_{\mathbf{k}}(\mathbf{x}) \sim e^{i\mathbf{k}\cdot\mathbf{x}}$, labeled by the wave vector \mathbf{k} .

$$|\mathbf{k}\rangle = \int d\mathbf{x} \psi_{\mathbf{k}}(\mathbf{x}) |\mathbf{x}\rangle = \frac{1}{V^{1/2}} \int d\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}} |\mathbf{x}\rangle. \quad (260)$$

- V - volume of the system, to provide appropriate normalization for the wave function.

When the electron is moving in a crystal, it also experience the *potential energy* from the lattice background

$$H = H_0 + \int d\mathbf{x} |\mathbf{x}\rangle V(\mathbf{x}) \langle \mathbf{x}|. \quad (261)$$

- A key feature is that $V(\mathbf{x})$ is *periodic*

$$V(\mathbf{x}) = V(\mathbf{x} + \mathbf{R}), \quad (262)$$

where \mathbf{R} is *any* lattice vector. Because atoms are arranged on a periodic lattice in the crystal.

- Transform the potential energy to the momentum space

$$\int d\mathbf{x} |\mathbf{x}\rangle V(\mathbf{x}) \langle \mathbf{x}| = \sum_{\mathbf{k}, \mathbf{k}'} |\mathbf{k}'\rangle V_{\mathbf{k}' - \mathbf{k}} \langle \mathbf{k}|, \quad (263)$$

with $V_{\mathbf{q}}$ being the Fourier transform of $V(\mathbf{x})$

$$V_{\mathbf{q}} = \frac{1}{V} \int d\mathbf{x} V(\mathbf{x}) e^{-i \mathbf{q} \cdot \mathbf{x}}. \quad (264)$$

Exc 11 | Derive Eq. (263).

- However, the periodicity of $V(\mathbf{x})$ in Eq. (262) puts a strong constraint on its Fourier transform $V_{\mathbf{q}}$ in Eq. (264) that

$$V_{\mathbf{q}} = e^{-i \mathbf{q} \cdot \mathbf{R}} V_{\mathbf{q}}, \quad (266)$$

for *any* lattice vector \mathbf{R} . For this equation to hold,

- Either \mathbf{q} satisfies the condition $\forall \mathbf{R}: e^{-i \mathbf{q} \cdot \mathbf{R}} = 1$, i.e. $\mathbf{q} = \mathbf{G} \in$ reciprocal lattice.
- Or \mathbf{q} is not on the reciprocal lattice, then $V_{\mathbf{q}} = 0$ must vanish.

This means

$$V_{\mathbf{q}} = \sum_{\mathbf{G}} V_{\mathbf{G}} \delta(\mathbf{q} - \mathbf{G}). \quad (267)$$

Then the full Hamiltonian reads

$$H = \sum_{\mathbf{k}} \left(|\mathbf{k}\rangle \frac{\hbar^2 \mathbf{k}^2}{2m} \langle \mathbf{k}| + \sum_{\mathbf{G}} |\mathbf{k} + \mathbf{G}\rangle V_{\mathbf{G}} \langle \mathbf{k}| \right). \quad (268)$$

with

- \mathbf{G} is summed over all reciprocal vectors on the reciprocal lattice,
- $V_{\mathbf{G}}$ describes the **scattering strength** that an electron is scattered from momentum $\hbar \mathbf{k}$ to $\hbar(\mathbf{k} + \mathbf{G})$ on the lattice, and is given by

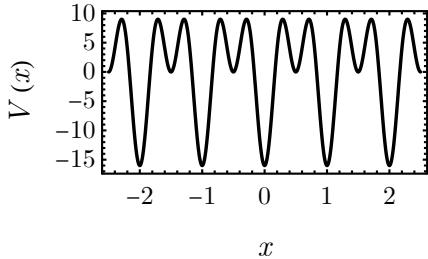
$$V_G = \frac{1}{V} \int d\mathbf{x} V(\mathbf{x}) e^{-i \mathbf{G} \cdot \mathbf{x}}. \quad (269)$$

- The $|\mathbf{k}\rangle$ state can only be mixed with $|\mathbf{k} + \mathbf{G}\rangle$ states related by the lattice momentum. This is a manifestation of the **Laue condition** (the conservation of quasi-momentum).

■ Electron in 1D Periodic Potential

Consider a 1D periodic potential

$$V(x) = V_0 + 2 V_1 \cos(2\pi x) + 2 V_2 \cos(4\pi x). \quad (270)$$



- Lattice constant $a = 1 \Rightarrow$ Reciprocal lattice constant $b = 2\pi/a = 2\pi \Rightarrow$ Reciprocal lattice vectors $G_m = m b = 2\pi m$ ($m \in \mathbb{Z}$ - the Miller index, not the electron mass)
- Scattering strength

$$V_G = \begin{cases} V_0 & G = 0 \\ V_1 & G = \pm 2\pi \\ V_2 & G = \pm 4\pi \\ 0 & \text{otherwise} \end{cases}, \quad (271)$$

- Takes the set of basis states given a momentum $k \in \text{BZ}$ in the *first Brillouin zone*

$$\dots, |k-4\pi\rangle, |k-2\pi\rangle, |k\rangle, |k+2\pi\rangle, |k+4\pi\rangle, \dots \quad (272)$$

the Hamiltonian can be represented as a matrix

$$H_k = \begin{pmatrix} \ddots & \ddots & \ddots & & & \\ \ddots & \xi_{k-4\pi} & V_1 & V_2 & & \\ \ddots & V_1 & \xi_{k-2\pi} & V_1 & V_2 & \\ & V_2 & V_1 & \xi_k & V_1 & V_2 \\ & & V_2 & V_1 & \xi_{k+2\pi} & V_1 & \ddots \\ & & & V_2 & V_1 & \xi_{k+4\pi} & \ddots \\ & & & & \ddots & \ddots & \ddots \end{pmatrix}, \quad (273)$$

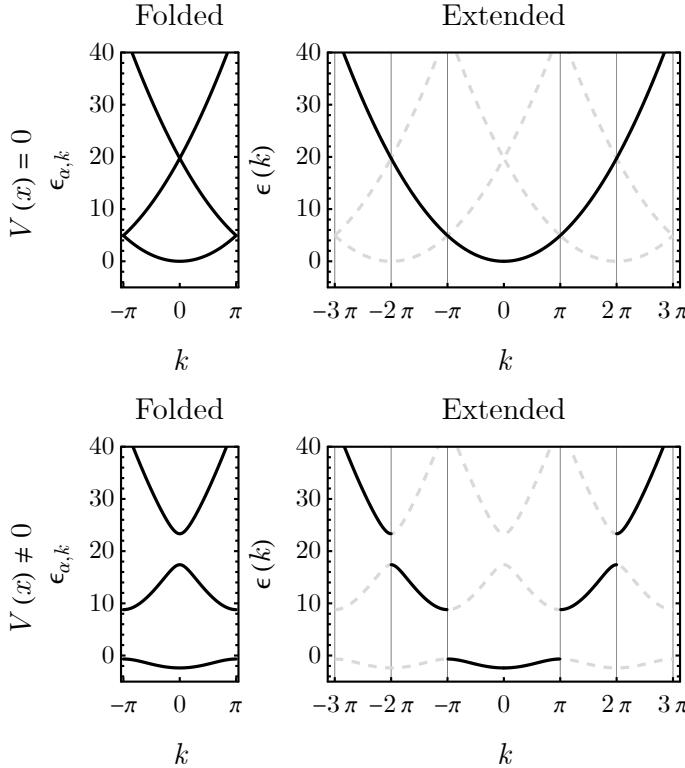
where the diagonal energy is given by

$$\xi_k = \frac{\hbar^2 k^2}{2m} + V_0. \quad (274)$$

- Diagonalize the Hamiltonian to find the eigen energies and eigenstates

$$H_k |\alpha, k\rangle = \epsilon_{\alpha,k} |\alpha, k\rangle. \quad (275)$$

- **α - band index**, labels the n th eigen state of H_k at each k
- **k - quasi-momentum**, there is no need to take k out side the *first Brillouin zone* as that do not leads to a new set of basis states.
- $\epsilon_{\alpha,k}$ - **dispersion relation** of the α th energy band (corresponds to the n th eigenvalue of H_k)

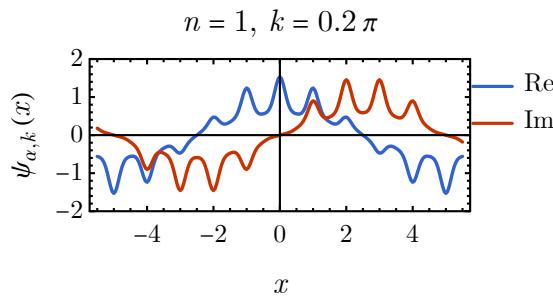


- **Band gap** opens at the Brillouin zone boundary.
- The dispersion can be unfolded to extended Brillouin zones following $\epsilon_{\alpha,k} \rightarrow \epsilon(k - 2\pi(-)^{\alpha} \lfloor \frac{\alpha}{2} \rfloor \text{sgn}(k))$.
- $|\alpha, k\rangle$ - eigenstate, as a linear combination of basis states

$$|\alpha, k\rangle = \sum_{m \in \mathbb{Z}} \tilde{u}_{\alpha, k, 2\pi m} |k+2\pi m\rangle, \quad (276)$$

in real space basis

$$\psi_{\alpha,k}(x) = \langle x | \alpha, k \rangle = \sum_{m \in \mathbb{Z}} \tilde{u}_{\alpha, k, 2\pi m} e^{i(k+2\pi m)x}, \quad (277)$$

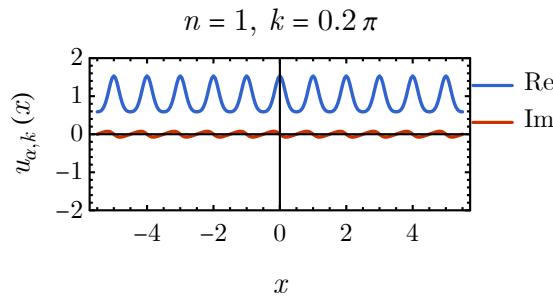


- Every eigenstate is a plane wave e^{ikx} modulated by a periodic function $u_{\alpha,k}(x)$ (in response to the periodic potential). $u_{\alpha,k}(x)$ is called the **Bloch function**, defined as

$$u_{\alpha,k}(x) = \sum_{m \in \mathbb{Z}} \tilde{u}_{\alpha,k,2\pi m} e^{i 2\pi m x}, \quad (278)$$

such that Eq. (277) explicitly takes the form of

$$\psi_{\alpha,k}(x) = u_{\alpha,k}(x) e^{i k x}. \quad (279)$$



- The Bloch function is periodic in x . Because if x is shifted by a lattice vector $x \rightarrow x + n$ ($n \in \mathbb{Z}$), by definition, we have

$$\begin{aligned} u_{\alpha,k}(x+n) &= \sum_{m \in \mathbb{Z}} \tilde{u}_{\alpha,k,2\pi m} e^{i 2\pi m x} e^{i 2\pi m n} \\ &= \sum_{m \in \mathbb{Z}} \tilde{u}_{\alpha,k,2\pi m} e^{i 2\pi m x} = u_{\alpha,k}(x). \end{aligned} \quad (280)$$

**HW
5**

In the near free electron model, calculate the effective mass of electron at the boundary between the m th and $(m+1)$ th Brillouin zone (where the band gap opens). [Hint: focus on the $|k=\pm m\pi\rangle$ states and apply the 2nd order perturbation theory].

Solution (HW 5)

■ Bloch Theorem

Bloch theorem: An electron in a *periodic* potential $V(\mathbf{x}) = V(\mathbf{x} + \mathbf{R})$ has *eigenstates* of the form

$$\psi_{\alpha,k}(\mathbf{x}) = \langle \mathbf{x} | \alpha, \mathbf{k} \rangle = u_{\alpha,k}(\mathbf{x}) e^{i k \cdot \mathbf{x}}, \quad (288)$$

where the *Bloch function* $u_{\alpha,k}(\mathbf{x}) = u_{\alpha,k}(\mathbf{x} + \mathbf{R})$ is *periodic* in \mathbf{x} (with the same periodicity as the potential), and the *quasi-momentum* \mathbf{k} is chosen within the first Brillouin zone.

- Proof: in the Hamiltonian Eq. (268), because the scattering term $\sum_{\mathbf{G}} |\mathbf{k} + \mathbf{G}\rangle V_{\mathbf{G}} \langle \mathbf{k}|$ only connects momentum eigenstates $|\mathbf{k}\rangle$ and $|\mathbf{k} + \mathbf{G}\rangle$ that are related by the reciprocal lattice vector \mathbf{G} . So the energy eigenstates (eigenstates of H) must be a linear combination of these momentum eigenstates, with some combination coefficients $\tilde{u}_{\alpha,k,G}$

$$|\alpha, \mathbf{k}\rangle = \sum_{\mathbf{G}} \tilde{u}_{\alpha,k,G} |\mathbf{k} + \mathbf{G}\rangle, \quad (289)$$

where α is the band index (labeling the α th eigenstate of H). In real space basis,

$$\begin{aligned} \langle \mathbf{x} | \alpha, \mathbf{k} \rangle &= \sum_{\mathbf{G}} \tilde{u}_{\alpha,k,G} \langle \mathbf{x} | \mathbf{k} + \mathbf{G} \rangle \\ &= \sum_{\mathbf{G}} \tilde{u}_{\alpha,k,G} e^{i(k+G) \cdot x} \\ &= u_{\alpha,k}(\mathbf{x}) e^{i k \cdot x}, \end{aligned} \quad (290)$$

where the Bloch function $u_{\alpha,k}(\mathbf{x})$ is introduced as the Fourier transform of the coefficients $\tilde{u}_{\alpha,k,G}$,

$$u_{\alpha,k}(\mathbf{x}) = \sum_{\mathbf{G}} \tilde{u}_{\alpha,k,G} e^{i G \cdot x}, \quad (291)$$

which must be periodic in \mathbf{x} , as

$$u_{\alpha,k}(\mathbf{x} + \mathbf{R}) = \sum_{\mathbf{G}} \tilde{u}_{\alpha,k,G} e^{i G \cdot x} e^{i G \cdot R} = u_{\alpha,k}(\mathbf{x}), \quad (292)$$

given that $e^{i G \cdot R} = 1$ by definition of the reciprocal lattice.

- \mathbf{k} is called the *quasi-momentum* because $|\alpha, \mathbf{k}\rangle$ state is a superposition of different momentum eigenstates, that does not have a definite momentum, but it labels a equivalent class of momenta that are all related by the Laue condition.

$$\begin{array}{ccc} |\alpha, \mathbf{k}\rangle & = \sum_{\mathbf{G}} \tilde{u}_{\alpha,k,G} & |\mathbf{k} + \mathbf{G}\rangle \\ \uparrow & & \uparrow \\ \text{quasi-momentum} & & \text{true momentum} \end{array} \quad (293)$$

- The electron still propagates in the form of a (modulated) *plane wave* in the crystal, with a *quasi-momentum*, similar to the plane wave state of a free electron.

Even though the potential that the electron feels from each atom is extremely strong, the electrons will still behave *almost* as if they do not see the atoms at all!

When I started to think about it, I felt that the main problem was to explain how the electrons could sneak by all the ions in a metal so as to avoid a mean free path of the order of atomic distance ... By straight Fourier analysis I found to my delight that the wave differed from the plane wave of

free electrons only by a periodic modulation.

— Felix Bloch (1952 Nobel Prize)

■ Equation of Motion for Bloch Electron

A *free electron* in an *electric field*

- *Classical* mechanics (Newton's 2nd law)

$$\frac{d\mathbf{p}}{dt} = \mathbf{F} = -e \mathbf{E}. \quad (294)$$

- *Quantum* mechanics (Schrödinger equation)

$$i\hbar \partial_t \psi = H \psi, \quad (295)$$

formal solution:

$$\psi \rightarrow e^{-\frac{i}{\hbar} H t} \psi, \quad (296)$$

the electron matter wave will accumulate the phase in *time* in the rate that is set by the *energy*.

The potential energy of an electron in the electric field is

$$V(\mathbf{x}) = e \mathbf{E} \cdot \mathbf{x}. \quad (297)$$

A plane wave state $|\mathbf{k}\rangle$ will evolve in the electric field as

$$e^{i\mathbf{k}\cdot\mathbf{x}} \rightarrow e^{-\frac{i}{\hbar} V(\mathbf{x}) t} e^{i\mathbf{k}\cdot\mathbf{x}} = e^{i\left(\mathbf{k} - \frac{1}{\hbar} e \mathbf{E} t\right) \cdot \mathbf{x}}, \quad (298)$$

meaning that the momentum $\hbar \mathbf{k}$ of the electron will change in time as

$$\hbar \mathbf{k} \rightarrow \hbar \mathbf{k} - e \mathbf{E} t, \quad (299)$$

or described by

$$\frac{d(\hbar \mathbf{k})}{dt} = -e \mathbf{E}, \quad (300)$$

matching the classical mechanics result.

For a **Bloch electron** (electron in a crystal)

$$|\alpha, \mathbf{k}\rangle = \sum_{\mathbf{G}} \tilde{u}_{\alpha, \mathbf{k}, \mathbf{G}} |\mathbf{k} + \mathbf{G}\rangle, \quad (301)$$

in the presence of the electric field \mathbf{E} , every (actual) momentum eigenstate $|\mathbf{k}\rangle$ will evolve in time as

$$|\mathbf{k}\rangle \rightarrow |\mathbf{k} - (e/\hbar) \mathbf{E} t\rangle. \quad (302)$$

Therefore the Bloch state evolves as (assuming $(e/\hbar) E t \ll 2\pi$, such that $\tilde{u}_{\alpha, \mathbf{k}, \mathbf{G}}$ remains approximately the same)

$$|\alpha, \mathbf{k}\rangle \rightarrow \sum_{\mathbf{G}} \tilde{u}_{\alpha, \mathbf{k}, \mathbf{G}} |\mathbf{k} - (e/\hbar) \mathbf{E} t + \mathbf{G}\rangle$$

$$\begin{aligned} &\simeq \sum_{\mathbf{G}} \tilde{u}_{\alpha, \mathbf{k} - (e/\hbar) \mathbf{E} t, \mathbf{G}} |\mathbf{k} - (e/\hbar) \mathbf{E} t + \mathbf{G}\rangle \\ &= |\alpha, \mathbf{k} - (e/\hbar) \mathbf{E} t\rangle, \end{aligned}$$

meaning that the *quasi-momentum* also satisfies Newton's 2nd law

$$\boxed{\frac{d(\hbar \mathbf{k})}{dt} = -e \mathbf{E} = \mathbf{F}.} \quad (304)$$

Metal (Fermi Gas) Phase

■ Thermodynamic Properties

■ Fermi-Dirac Distribution

Electron is a fermion. Its finite-temperature behavior is determined by the Fermi-Dirac distribution.

- **Pauli exclusion principle.** A fermion mode can either be *empty* or *occupied* by *one* fermion, but not occupied by multiple fermions.

Consider a system containing only one fermion mode. Let n be the **occupation number** of the fermion mode

$$n = \begin{cases} 0 & \text{empty} \\ 1 & \text{occupied} \end{cases}. \quad (305)$$

- Total **energy** of the system

$$E = \epsilon n = \begin{cases} 0 & \text{empty} \\ \epsilon & \text{occupied} \end{cases}. \quad (306)$$

- Total **fermion number** of the system

$$N = n = \begin{cases} 0 & \text{empty} \\ 1 & \text{occupied} \end{cases}. \quad (307)$$

- Probability to observe the system in the state with occupation number n is

$$p_n = \frac{1}{Z} e^{-\beta(E-\mu N)} = \frac{1}{Z} e^{-\beta(\epsilon-\mu) n}, \quad (308)$$

where Z is the partition function (quantum, grand canonical ensemble)

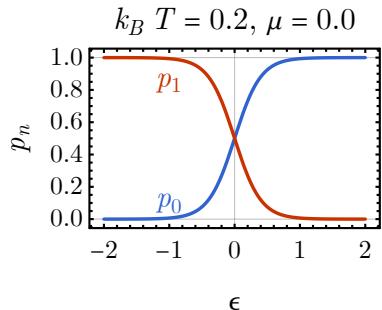
$$Z = \sum_{n=0,1} e^{-\beta(\epsilon-\mu) n} = 1 + e^{-\beta(\epsilon-\mu)}. \quad (309)$$

- $\beta = 1/(k_B T)$: k_B - Boltzmann constant, T - temperature.

- μ - chemical potential.

More explicitly

$$p_0 = \frac{1}{1 + e^{-\beta(\epsilon-\mu)}}, \quad p_1 = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}. \quad (310)$$



- Average occupation number

$$\langle n \rangle = \sum_{n=0,1} n p_n = p_1 = n_F(\beta(\epsilon - \mu)), \quad (311)$$

where n_F is the **Fermi-Dirac distribution** function

$$n_F(\beta(\epsilon - \mu)) = \frac{1}{e^{\beta(\epsilon - \mu)} + 1}. \quad (312)$$

describing the average number of fermions occupying the mode of energy ϵ .

- Average energy

$$\begin{aligned} \langle E \rangle &= \sum_{n=0,1} E p_n \\ &= \epsilon n_F(\beta(\epsilon - \mu)). \end{aligned} \quad (313)$$

- Average fermion (electron) number

$$\begin{aligned} \langle N \rangle &= \sum_{n=0,1} N p_n \\ &= n_F(\beta(\epsilon - \mu)). \end{aligned} \quad (314)$$

Note: Here $\langle N \rangle = \langle n \rangle$ because the system has only one single mode.

■ Fermi Energy

Metal phase is formed by many (weakly interacting) electrons that partially fill a band. The band structure (near the Γ point) can be described by the **quadratic dispersion**

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2 m_{\text{eff}}}, \quad (315)$$

- m_{eff} - effective mass of electron in the crystal.
- \mathbf{k} - quasi-momentum. Each \mathbf{k} labels a mode $|\mathbf{k}\rangle$ that can be occupied by the electron. More precisely, the electron also carries spin, that can be in one of the two degenerated spin states, so the electronic mode is jointly labeled by $|\mathbf{k}, \sigma\rangle$ ($\sigma = \uparrow, \downarrow$).

The average total number of electron

$$\begin{aligned} N &= 2 \sum_{\mathbf{k}} n_{\text{F}}(\beta(\epsilon_{\mathbf{k}} - \mu)) \\ &= 2 \frac{V}{(2\pi)^D} \int d^D \mathbf{k} n_{\text{F}}(\beta(\epsilon_{\mathbf{k}} - \mu)). \end{aligned} \quad (316)$$

- Prefactor of 2 accounts for the two degenerated spin states (the ways that electrons occupy both spins states are identical).
- D - dimension of space.
- V - volume of the system. Such that the discretization unit in the momentum space is $(2\pi)^D / V$.

Define: **Fermi energy** (or Fermi level) ϵ_{F} of the electronic system to be the *chemical potential* at zero temperature $T = 0$ limit, given the number of electrons in the system.

- **Fermi temperature** T_{F}

$$k_B T_{\text{F}} = \epsilon_{\text{F}}. \quad (317)$$

- **Fermi momentum** k_{F}

$$\frac{\hbar^2 k_{\text{F}}^2}{2 m_{\text{eff}}} = \epsilon_{\text{F}}. \quad (318)$$

- **Fermi velocity** v_{F}

$$v_{\text{F}} = \frac{\hbar k_{\text{F}}}{m_{\text{eff}}}, \quad (319)$$

hence $\epsilon_{\text{F}} = \frac{1}{2} m_{\text{eff}} v_{\text{F}}^2$.

- Number of electrons at $T = 0$. At zero temperature, the Fermi-Dirac distribution function reduces to a step function (written as $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ for $x < 0$), such that Eq. (316) becomes

$$\begin{aligned} N &= 2 \frac{V}{(2\pi)^D} \int d^D \mathbf{k} \Theta(\epsilon_{\text{F}} - \epsilon_{\mathbf{k}}), \\ &= 2 \frac{V}{(2\pi)^D} \int^{k < k_{\text{F}}} d^D \mathbf{k} \end{aligned}$$

$$= 2 \frac{V}{(2\pi)^D} \int_{k=0}^{k=k_F} A_D k^{D-1} dk$$

$$= 2 \frac{V A_D k_F^D}{D (2\pi)^D},$$

- $A_D = 2\pi^{D/2} / \Gamma\left(\frac{D}{2}\right)$ - area of a $(D-1)$ -dimensional unit sphere (in the D -dimensional space).
 $A_D k_F^D / D$ is the volume of a ball of radius k_F .
- At $T = 0$, the electrons simply fill a ball in the momentum space of radius k_F . The surface is the ball is called the **Fermi surface**.
- From Eq. (320), we can solve for the Fermi momentum k_F

$$k_F = 2\pi \left(\frac{D}{2A_D} \frac{N}{V} \right)^{1/D} \quad (321)$$

or more explicitly (let $n = N / V$)

$$k_F = \begin{cases} \pi n / 2 & D = 1 \\ (2\pi n)^{1/2} & D = 2 \\ (3\pi^2 n)^{1/3} & D = 3 \\ \dots & \dots \end{cases}. \quad (322)$$

- Correspondingly the Fermi energy

$$\epsilon_F = \frac{(2\pi)^2 \hbar^2}{2 m_{\text{eff}}} \left(\frac{D}{2A_D} \frac{N}{V} \right)^{2/D}. \quad (323)$$

or more explicitly (let $n = N / V$)

$$\epsilon_F = \frac{\hbar^2}{2 m_{\text{eff}}} \begin{cases} (\pi n / 2)^2 & D = 1 \\ 2\pi n & D = 2 \\ (3\pi^2 n)^{2/3} & D = 3 \\ \dots & \dots \end{cases}. \quad (324)$$

- For typical metals, the Fermi energy is of the order $\epsilon_F \sim 10 \text{ eV}$, which corresponds to a Fermi temperature of the order $T_F \sim 10^5 \text{ K}$, much higher than the room temperature (also much higher than the melting temperature of metals).

Therefore, most electrons in the metal are deep in the Fermi sea and do not participate in thermodynamic or transport process. Such many-body state of electrons is also called **degenerate Fermi gas**, which also happens in other fermion systems as long as $T \ll T_F$ (cold atomic gas $T_F \sim 10^{-6} \text{ K}$, white dwarf star $T_F \sim 10^9 \text{ K}$).

- For typical metals, the Fermi velocity can be as large as $v_F \sim 0.01 c$ (c - the speed of light). The high velocity of electron originated from the Pauli exclusion principle — all low momentum (low velocity) states are filled, and the active electrons around the Fermi surface has to move with high velocity.

■ Density of States

At finite temperature, the average total energy E and total number N of electrons is given by

$$\begin{aligned} E &= 2 \sum_k \epsilon_k n_F(\beta(\epsilon_k - \mu)), \\ N &= 2 \sum_k n_F(\beta(\epsilon_k - \mu)). \end{aligned} \quad (325)$$

The momentum summation can be converted to an energy integration

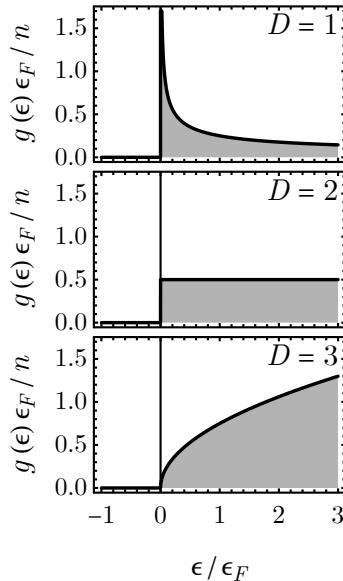
$$\sum_k = \frac{V}{(2\pi)^D} \int d^D k = V \int d\epsilon_k g(\epsilon_k), \quad (326)$$

by introducing the **density of states**

$$g(\epsilon) = \frac{D n}{4 \epsilon_F} \left(\frac{\epsilon}{\epsilon_F} \right)^{D/2-1} \Theta(\epsilon), \quad (327)$$

**Exc
12**

Derive Eq. (327).



Using Eq. (326), Eq. (325) can be written as

$$\begin{aligned} E &= 2 V \int d\epsilon g(\epsilon) \epsilon n_F(\beta(\epsilon - \mu)), \\ N &= 2 V \int d\epsilon g(\epsilon) n_F(\beta(\epsilon - \mu)). \end{aligned} \quad (331)$$

HW 6 If the band structure has a linear dispersion (as for Dirac fermions) $\epsilon_{k,\pm} = \pm \hbar v_F |\mathbf{k}|$, calculate the density of state $g(\epsilon)$ in general D -dimensional space.

Solution (HW 6)

■ Low-Temperature Expansion

Both integrals in Eq. (331) are of the form

$$I = \int_{-\infty}^{\mu} d\epsilon f(\epsilon) n_F(\beta(\epsilon - \mu)). \quad (334)$$

which admits the **low-temperature expansion** (Sommerfeld expansion) as $T \rightarrow 0$,

$$I = \int_{-\infty}^{\mu} d\epsilon f(\epsilon) + \sum_{n=1}^{\infty} \frac{2(k_B T)^{2n}}{(2n-1)!} \partial_{\mu}^{2n-1} f(\mu) I_{2n-1}, \quad (335)$$

where the constants are given by

$$I_{2n-1} = \int_0^{\infty} \frac{x^{2n-1}}{e^x + 1} dx = \left(1 - \frac{2}{4^n}\right) \Gamma(2n) \zeta(2n). \quad (336)$$

Exc 13 Derive Eq. (335) and Eq. (336).

The leading terms of the expansion reads

$$\int_{-\infty}^{\mu} d\epsilon f(\epsilon) n_F(\beta(\epsilon - \mu)) = \int_{-\infty}^{\mu} d\epsilon f(\epsilon) + \frac{(\pi k_B T)^2}{6} f'(\mu) + \dots \quad (341)$$

Using Eq. (341), Eq. (331) can be evaluated to the leading order of T

$$\begin{aligned} E(\mu, T) &= \frac{D}{D+2} N \epsilon_F + 2(\mu - \epsilon_F) g(\epsilon_F) \epsilon_F V + \frac{(\pi k_B T)^2}{3} (g(\mu) + \mu g'(\mu)) V + \dots, \\ N(\mu, T) &= N + 2(\mu - \epsilon_F) g(\epsilon_F) V + \frac{(\pi k_B T)^2}{3} g'(\mu) V + \dots. \end{aligned} \quad (342)$$

Exc 14 Derive Eq. (342).

The second equation (regarding N) in Eq. (342) implies that the chemical potential μ must vary with the temperature T in the following manner to keep the particle number fixed

$$\mu = \epsilon_F - \frac{(\pi k_B T)^2}{6} \frac{g'(\epsilon_F)}{g(\epsilon_F)}. \quad (347)$$

Substitute Eq. (347) into Eq. (342), we obtain the energy of the degenerate Fermi gas at low temperature

$$E(T) = \frac{D}{D+2} N \epsilon_F + \frac{(\pi k_B T)^2}{3} g(\epsilon_F) V + \dots \quad (348)$$

HW 7 If the density of state respects the particle-hole symmetry $g(\epsilon) = g(-\epsilon)$ (as in graphene), prove that if at zero temperature the Fermi energy is at $\epsilon_F = 0$, then the chemical potential is locked at zero $\mu(T) = 0$ for any finite temperature.

Solution (HW 7)

■ Heat Capacity

- **Heat capacity:** the rate of energy E change with respect to the temperature T

$$C_V = \frac{\partial E}{\partial T} = \frac{\pi^2 k_B^2 T}{3} (2 g(\epsilon_F) V). \quad (352)$$

For quadratic dispersion, the density of state $g(\epsilon)$ given in Eq. (327),

$$C_V = \frac{\pi^2}{3} \left(\frac{D N k_B}{2} \right) \left(\frac{T}{T_F} \right). \quad (353)$$

- **Specific heat:** heat capacity per electron

$$c_V = \frac{C_V}{N} = \frac{\pi^2 k_B^2 T}{3} \frac{2 g(\epsilon_F)}{n}. \quad (354)$$

For quadratic dispersion

$$c_V = \frac{\pi^2}{3} \left(\frac{D k_B}{2} \right) \left(\frac{T}{T_F} \right). \quad (355)$$

- $D k_B / 2$ is the classical result for specific heat of a gas, where every atom in the gas can exchange energy with the heat bath. However, in metals, on those electrons near the Fermi surface can absorb/release energy, so the specific heat of such degenerate Fermi gas is smaller than the classical gas by a factor of T / T_F , which is a tiny ratio $T / T_F \sim 0.01$ in typical metals.

- At low-temperature, the specific heat of electrons in metals grows with temperature linearly $c_V \sim T$ (regardless of the spatial dimension D of the system).

Further taken into account the specific heat of phonons, which scales as $c_V \sim T^D$, the total specific heat should take the form of

$$c_V = \gamma T + \alpha T^D, \quad (356)$$

for D -dimensional metal at low-temperature.

**HW
8**

Show that the electronic contribution to the specific heat in a single-layer graphene scales as $c_V \sim T^2$ at low temperature. [Hint: consider the low-energy electrons in graphene as 2D Dirac fermions with linear dispersion.]

Solution (HW 8)

■ Charge Compressibility

- **Charge compressibility** (quantum capacitance): the rate of charge Q changes with respect to the electric potential U

$$C_Q = \frac{\partial Q}{\partial U} = e^2 \frac{\partial N}{\partial \mu}. \quad (363)$$

- e - electric charge of electron.
- In the presence of electric potential U , the electron chemical potential shifts by

$$\mu \rightarrow \mu - e U. \quad (364)$$

As a result the number of electron changes by

$$N \rightarrow N + \frac{\partial N}{\partial \mu} (-e U), \quad (365)$$

and the total charge $Q = -e N$ changes by

$$Q \rightarrow Q + e^2 \frac{\partial N}{\partial \mu} U. \quad (366)$$

- Using the result in Eq. (342),

$$N(\mu, T) = N + 2(\mu - \epsilon_F) g(\epsilon_F) V + \dots, \quad (367)$$

we have

$$\frac{\partial N}{\partial \mu} = 2 g(\epsilon_F) V. \quad (368)$$

So the charge compressibility is given by

$$C_Q = e^2 \frac{\partial N}{\partial \mu} = e^2 (2 g(\epsilon_F) V). \quad (369)$$

For quadratic dispersion, the density of state $g(\epsilon)$ given in Eq. (327),

$$C_Q = \frac{e^2 D N}{2 \epsilon_F} \quad (370)$$

- Specific charge compressibility

$$c_Q = \frac{C_Q}{N} = e^2 \frac{2 g(\epsilon_F)}{n}. \quad (371)$$

For quadratic dispersion,

$$c_Q = \frac{e^2 D}{2 \epsilon_F}. \quad (372)$$

■ Spin Susceptibility

- Spin susceptibility: the rate of magnetization M changes with respect to the external magnetic field B

$$\chi = \frac{\partial M}{\partial B} \quad (373)$$

- $\mu_B = e \hbar / (2 m_e)$ - **Bohr magneton**, the magnetic moment carried by the electron.
- In the presence of a magnetic field B , the up-spin and down-spin electron energy split

$$\begin{aligned} \epsilon_{k,\uparrow} &= \epsilon_k + \mu_B B, \\ \epsilon_{k,\downarrow} &= \epsilon_k - \mu_B B. \end{aligned} \quad (374)$$

Magnetization (average magnetic moment per electron) responds to the magnetic field as

$$\begin{aligned} M &= \mu_B \frac{N_\uparrow - N_\downarrow}{N} \\ &= \frac{\mu_B}{N} \left(\frac{\partial N_\uparrow}{\partial \mu_\uparrow} (\mu_B B) - \frac{\partial N_\downarrow}{\partial \mu_\downarrow} (-\mu_B B) \right) \\ &= \frac{\mu_B^2}{N} \left(\frac{\partial N_\uparrow}{\partial \mu_\uparrow} + \frac{\partial N_\downarrow}{\partial \mu_\downarrow} \right) B \\ &= \frac{\mu_B^2}{N} \frac{\partial N}{\partial \mu} B. \end{aligned} \quad (375)$$

So the spin susceptibility can be calculated as

$$\chi = \frac{\mu_B^2}{N} \frac{\partial N}{\partial \mu} = \mu_B^2 \frac{2 g(\epsilon_F)}{n}. \quad (376)$$

For quadratic dispersion, the density of state $g(\epsilon)$ given in Eq. (327),

$$\chi = \frac{\mu_B^2 D}{2 \epsilon_F}. \quad (377)$$

This constant spin susceptibility of the electron gas is also called the **Pauli susceptibility**, which (partially) explains the **paramagnetism** of metal.

■ Wilson Ratio

Specific heat c_V , charge compressibility c_Q , and spin susceptibility χ are all proportional to $2 g(\epsilon_F) / n$:

$$\begin{aligned} c_V &= \frac{\pi^2 k_B^2 T}{3} \frac{2 g(\epsilon_F)}{n}, \\ c_Q &= e^2 \frac{2 g(\epsilon_F)}{n}, \\ \chi &= \mu_B^2 \frac{2 g(\epsilon_F)}{n}. \end{aligned} \quad (378)$$

By taking ratios among them, the non-universal property $2 g(\epsilon_F) / n$ can be canceled. The resulting universal ratio is called the **Wilson ratio**,

$$R_W = \frac{c_Q T}{c_V} \frac{\pi^2 k_B^2}{3 e^2} = \frac{\chi T}{c_V} \frac{\pi^2 k_B^2}{3 \mu_B^2} = 1. \quad (379)$$

- For non-interacting electrons, the Wilson ratio should be 1, which is expected to hold for typical metals.
- Deviation of the Wilson ratio from unity signifies the interaction effect between electrons is important in the material.

■ Transport Properties

■ Boltzmann Transport

Transport properties concern how metal conduct electricity and heat. In order to generate electric/heat current in the system, the electrons must deviate from their equilibrium distribution.

Boltzmann transport theory is a semiclassical theory for near-equilibrium electrons. The basic quantity of interest is the distribution function $f(\mathbf{x}, \mathbf{k}, t)$ of electron in the phase space (\mathbf{x}, \mathbf{k}) as a function of time t .

- **Equilibrium distribution.** Without external perturbations, electrons relax to the equilibrium distribution

$$f_{\text{eq}}(\mathbf{x}, \mathbf{k}) = n_F(\beta(\epsilon_k - \mu)) = \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1}. \quad (380)$$

At the low-temperature limit ($T \rightarrow 0$),

$$\begin{aligned} f_{\text{eq}}(\mathbf{x}, \mathbf{k}) &= \Theta(\epsilon_F - \epsilon_k) \\ \Rightarrow \frac{\partial f}{\partial \epsilon_k} &= -\delta(\epsilon_F - \epsilon_k). \end{aligned} \quad (381)$$

- Relaxation of near equilibrium distribution. If f deviated from f_{eq} , it will relax to f_{eq} in a characteristic time scale τ , called the **relaxation time**,

$$f(t) = f_{\text{eq}} + (f(0) - f_{\text{eq}}) e^{-t/\tau}. \quad (382)$$

The relaxation dynamics can be described by the following differential equation

$$\frac{df}{dt} = -\frac{f - f_{\text{eq}}}{\tau}. \quad (383)$$

- On the other hand, by the chain rule of differentiation

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{x}} \cdot \frac{d\mathbf{x}}{dt} + \frac{\partial f}{\partial \mathbf{k}} \cdot \frac{d\mathbf{k}}{dt}. \quad (384)$$

By semiclassical equation of motion

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \mathbf{v}_k = \frac{1}{\hbar} \partial_k \epsilon_k, \\ \frac{d\mathbf{k}}{dt} &= \frac{1}{\hbar} \mathbf{F}, \end{aligned} \quad (385)$$

- \mathbf{v}_k - group velocity of the electron at momentum \mathbf{k} ,
- \mathbf{F} - external force acting on the electron.

Eq. (384) can be written as

$$\frac{df}{dt} = \partial_t f + \mathbf{v}_k \cdot \partial_x f + \frac{1}{\hbar} \mathbf{F} \cdot \partial_k f. \quad (386)$$

Combine Eq. (383) and Eq. (386), we obtain the **Boltzmann equation**

$$\partial_t f + \mathbf{v}_k \cdot \partial_x f + \frac{1}{\hbar} \mathbf{F} \cdot \partial_k f = -\frac{f - f_{\text{eq}}}{\tau}. \quad (387)$$

The *stationary* solution is defined to be the solution that $\partial f / \partial t = 0$, which is given by

$$\mathbf{v}_k \cdot \partial_x f + \frac{1}{\hbar} \mathbf{F} \cdot \partial_k f = -\frac{f - f_{\text{eq}}}{\tau}. \quad (388)$$

■ Electrical Conductivity

Metal can conduct *electricity* in the presence of **electric field** \mathbf{E} . Electrons experience an external force

$$\mathbf{F} = -e \mathbf{E}. \quad (389)$$

Stationary solution should be given by Eq. (388)

$$-\frac{e}{\hbar} \mathbf{E} \cdot \partial_k f = -\frac{f - f_{\text{eq}}}{\tau}, \quad (390)$$

or written as a self-consistent equation

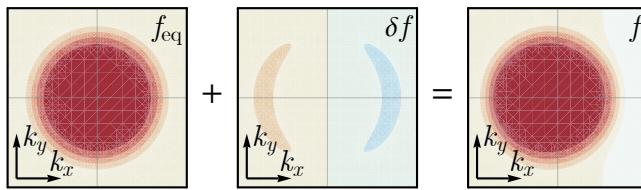
$$f = f_{\text{eq}} + \frac{e\tau}{\hbar} \mathbf{E} \cdot \partial_{\mathbf{k}} f. \quad (391)$$

Assuming f is close to f_{eq} , we can take $f \simeq f_{\text{eq}}$ as an initial approximation, and substitute it to Eq. (391) iteratively to find the self-consistent solution.

- To the first order in \mathbf{E} (linear response),

$$\begin{aligned} f &\simeq f_{\text{eq}} + \frac{e\tau}{\hbar} \mathbf{E} \cdot \partial_{\mathbf{k}} f_{\text{eq}} \\ &= f_{\text{eq}} + e\tau \mathbf{E} \cdot \mathbf{v}_{\mathbf{k}} \partial_{\epsilon} f_{\text{eq}}. \end{aligned} \quad (392)$$

- f is deviated from f_{eq} . The main effect is to *shift* the Fermi sea in the momentum space by the amount of $-(e\tau/\hbar)\mathbf{E}$.



This can induce an **electric current density**

$$\begin{aligned} \mathbf{J} &= -2e \int \frac{d^D \mathbf{k}}{(2\pi)^D} \mathbf{v}_{\mathbf{k}} f \\ &= -2e \int \frac{d^D \mathbf{k}}{(2\pi)^D} \mathbf{v}_{\mathbf{k}} f_{\text{eq}} - 2e^2 \tau \int \frac{d^D \mathbf{k}}{(2\pi)^D} \mathbf{v}_{\mathbf{k}} \mathbf{E} \cdot \mathbf{v}_{\mathbf{k}} \partial_{\epsilon} f_{\text{eq}}. \end{aligned} \quad (393)$$

- The prefactor 2 comes from the spin degeneracy
- The first term will vanish because there is no current when the system is at equilibrium.
- Switch the integral from the momentum space to the energy domain

$$\begin{aligned} \mathbf{J} &= -2e^2 \tau \int d\epsilon_{\mathbf{k}} g(\epsilon_{\mathbf{k}}) \mathbf{v}_{\mathbf{k}} \mathbf{E} \cdot \mathbf{v}_{\mathbf{k}} \partial_{\epsilon} f_{\text{eq}} \\ &= -\frac{2e^2 \tau v_F^2}{3} \mathbf{E} \int d\epsilon g(\epsilon) \partial_{\epsilon} f_{\text{eq}}. \end{aligned} \quad (394)$$

The integral admits the following low-temperature expansion

$$\int d\epsilon g(\epsilon) \partial_{\epsilon} f_{\text{eq}} = -g(\mu) - \frac{\pi^2}{6} \frac{\partial_{\mu}^2 g(\mu)}{\beta^2} + \dots, \quad (395)$$

Exc 15 | Derive Eq. (395).

Take the low-temperature limit and use $\mu = \epsilon_F$ as $T \rightarrow 0$,

$$\mathbf{J} = \frac{2e^2 \tau v_F^2}{3} g(\epsilon_F) \mathbf{E}. \quad (400)$$

The **electrical conductivity** σ is defined via

$$\mathbf{J} = \sigma \mathbf{E}. \quad (401)$$

Compare with Eq. (400), we can identify

$$\sigma = \frac{2 e^2 \tau v_F^2}{3} g(\epsilon_F). \quad (402)$$

Using the density of state $g(\epsilon)$ given in Eq. (327),

$$\sigma = \frac{D}{3} \frac{e^2 n \tau}{m_{\text{eff}}}. \quad (403)$$

■ Thermal Conductivity

Metal can conduct *heat* in the presence of **temperature gradient** $\partial_x T$ (heat will flow from the high temperature side to the low temperature side). The temperature gradient enters the Boltzmann equation by creating a spatial gradient of the distribution function

$$\partial_x f = \partial_T f \partial_x T. \quad (404)$$

Stationary solution should be given by Eq. (388)

$$\mathbf{v}_k \cdot \partial_x T \partial_T f = - \frac{f - f_{\text{eq}}}{\tau}, \quad (405)$$

or written as a self-consistent equation

$$f = f_{\text{eq}} - \tau \mathbf{v}_k \cdot \partial_x T \partial_T f. \quad (406)$$

Again, solving the self-consistent equation iteratively, starting from $f \simeq f_{\text{eq}}$.

- To the first order in $\partial_x T$ (linear response),

$$f \simeq f_{\text{eq}} - \tau \mathbf{v}_k \cdot \partial_x T \partial_T f_{\text{eq}}. \quad (407)$$

Given $f_{\text{eq}} = (e^{(\epsilon-\mu)/T} + 1)^{-1}$, $\partial_T f_{\text{eq}}$ and $\partial_\epsilon f_{\text{eq}}$ are related by

$$\partial_T f_{\text{eq}} = - \frac{\epsilon - \mu}{T} \partial_\epsilon f_{\text{eq}}, \quad (408)$$

therefore

$$f \simeq f_{\text{eq}} + \frac{\epsilon_k - \mu}{T} \tau \mathbf{v}_k \cdot \partial_x T \partial_\epsilon f_{\text{eq}}. \quad (409)$$

This can induced an **energy current density**

$$\mathbf{J}_Q = 2 \int \frac{d^D k}{(2\pi)^D} (\epsilon_k - \mu) \mathbf{v}_k f$$

$$= 2 \int \frac{d^D k}{(2\pi)^D} (\epsilon_k - \mu) v_k f_{\text{eq}} + 2 \int \frac{d^D k}{(2\pi)^D} \frac{(\epsilon_k - \mu)^2 \tau}{T} v_k \cdot \partial_x T \partial_\epsilon f_{\text{eq}}.$$

- The prefactor 2 comes from the spin degeneracy
- The first term will vanish because there is no current when the system is at equilibrium.
- Switch the integral from the momentum space to the energy domain

$$\begin{aligned} \mathbf{J}_Q &= \frac{2\tau}{T} \int \frac{d^D k}{(2\pi)^D} (\epsilon_k - \mu)^2 v_k \cdot \partial_x T \partial_\epsilon f_{\text{eq}} \\ &= \frac{2\tau}{T} \int d\epsilon_k g(\epsilon_k) (\epsilon_k - \mu)^2 v_k \cdot \partial_x T \partial_\epsilon f_{\text{eq}} \\ &= \frac{2\tau v_F^2}{3} \frac{\partial_x T}{T} \int d\epsilon g(\epsilon) (\epsilon - \mu)^2 \partial_\epsilon f_{\text{eq}}. \end{aligned} \quad (411)$$

Use the low-temperature expansion in Eq. (395)

$$\int d\epsilon g(\epsilon) (\epsilon - \mu)^2 \partial_\epsilon f_{\text{eq}} = -\frac{\pi^2}{3} \frac{g(\mu)}{\beta^2} + \dots, \quad (412)$$

therefore

$$\mathbf{J}_Q = -\frac{2\tau v_F^2}{3} g(\epsilon_F) \frac{\pi^2 k_B^2 T}{3} \partial_x T. \quad (413)$$

The **thermal conductivity** κ is defined via

$$\mathbf{J}_Q = -\kappa \partial_x T. \quad (414)$$

Compare with Eq. (413), we can identify

$$\begin{aligned} \kappa &= \frac{2\tau v_F^2}{3} g(\epsilon_F) \frac{\pi^2 k_B^2 T}{3} \\ &= \frac{\pi^2 k_B^2}{3 e^2} \sigma T \\ &= \frac{D}{3} \frac{\pi^2 k_B^2 n \tau}{3 m_{\text{eff}}} T, \end{aligned} \quad (415)$$

where σ is the electrical conductivity given in Eq. (402).

■ Lorenz Number

Eq. (415) reveals a proportionality between the thermal conductivity and the electrical conductivity, such that the ratio

$$L \equiv \frac{\kappa}{\sigma T} = \frac{\pi^2}{3} \left(\frac{k_B}{e} \right)^2 \approx 2.443 \times 10^{-8} \text{ W} \cdot \Omega \cdot \text{K}^{-2}, \quad (416)$$

is a universal constant, known as the **Lorenz number**.

Material	$L \times 10^8$
Sodium (Na)	2.12
Magnesium (Mg)	2.14
Copper (Cu)	2.20
Lithium (Li)	2.22
Zinc (Zn)	2.33
Silver (Ag)	2.37
Gold (Au)	2.40
Cadmium (Cd)	2.43
Lead (Pb)	2.56
Platinum (Pt)	2.60
Iron (Fe)	2.61
Tungsten (W)	3.20
Bismuth (Bi)	3.53

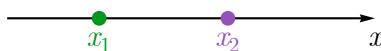
- The fact that many metals have roughly the same $\kappa/(\sigma T)$ ratio is also known as the **Wiedemann-Franz law**.
- Significance deviation of the Lorenz number of this value is an indication of the importance of electron interaction in the material.

Interacting Electrons

■ Interacting Two-Electron Systems

■ Warmup: Classical Interacting Particles

Consider two *classical* particles restricted in a 1D system, described by a pair of coordinates (x_1, x_2) .

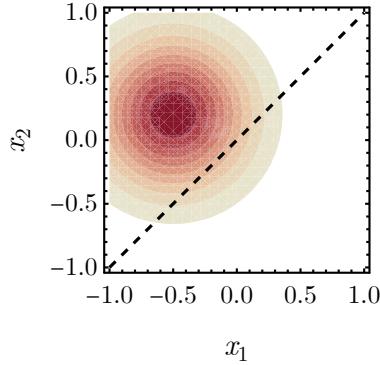


- Suppose there is some *uncertainty* about the positions → should think about the **probability distribution** of the particles $p(x_1)$ and $p(x_2)$



Or more precisely, the **joint probability distribution**

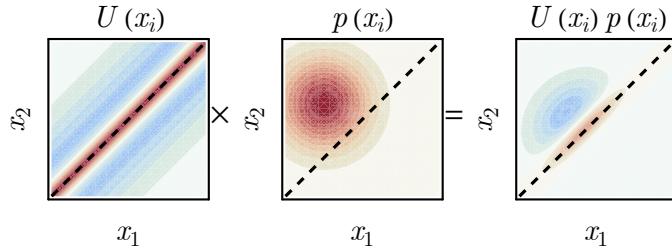
$$p(x_1, x_2) = p(x_1) p(x_2). \quad (417)$$



- Suppose the interaction between the two particles is described by the **interaction potential** $U(x_1 - x_2)$ (assuming translation symmetry and inversion symmetry), the *average interaction energy* is

$$E_U = \int dx_1 dx_2 U(x_1 - x_2) p(x_1, x_2). \quad (418)$$

(illustration of the integrand)



■ Interacting Fermions

However, the classical probability description does not apply to quantum particles, such as **fermions** (electrons).

- First, fermions are *identical* particles. There is no way to distinguish which electron is the first/second one. This implies that the probability distribution must be *invariant* under the *exchange* of the two fermions, i.e.

$$p(x_1, x_2) = p(x_2, x_1). \quad (419)$$

- Secondly, fermions are *quantum* particles. The probability $p(x_1, x_2)$ should be modeled by the underlying **probability amplitude** (the **wave function**) $\psi(x_1, x_2)$ as

$$p(x_1, x_2) = |\psi(x_1, x_2)|^2. \quad (420)$$

Then Eq. (419) requires

$$|\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2. \quad (421)$$

There are two options

$$\psi(x_1, x_2) = \begin{cases} +\psi(x_2, x_1) & \text{bosons,} \\ -\psi(x_2, x_1) & \text{fermions.} \end{cases} \quad (422)$$

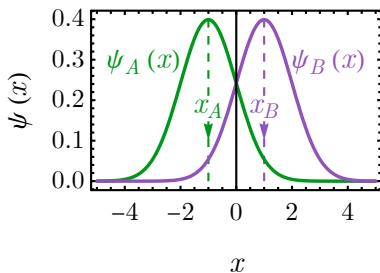
Definition: Bosons/Fermions are identical quantum particles, whose many-body wave functions are **symmetric/antisymmetric** under particle exchange.

Consider two fermions occupying $\psi_A(x)$ and $\psi_B(x)$ orbitals respectively, the two-body wave function must take the following form (to respect the fermion antisymmetry)

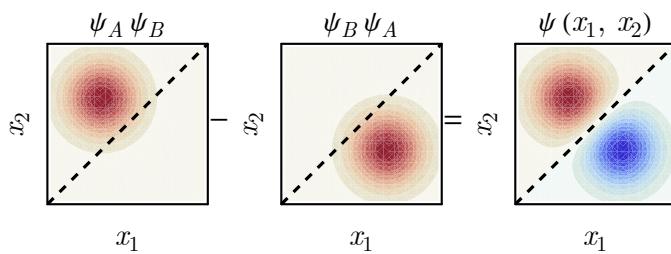
$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} (\psi_A(x_1) \psi_B(x_2) - \psi_B(x_1) \psi_A(x_2)). \quad (423)$$

- One can already see, if $\psi_A = \psi_B$ are the same state, the two-body wave function vanishes automatically \Rightarrow **Pauli exclusion principle**: fermions can not double occupy the same state.
- Consider two localized orbitals

$$\begin{aligned} \psi_A(x) &\propto \exp\left(-\frac{(x - x_A)^2}{2}\right), \\ \psi_B(x) &\propto \exp\left(-\frac{(x - x_B)^2}{2}\right). \end{aligned} \quad (424)$$



The two-body wave function can be constructed by antisymmetrization.



- Probability distribution

$$\begin{aligned} p(x_1, x_2) &= |\psi(x_1, x_2)|^2 \\ &= \frac{1}{2} |\psi_A(x_1) \psi_B(x_2) - \psi_B(x_1) \psi_A(x_2)|^2 \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{2} (|\psi_A(x_1)|^2 |\psi_B(x_2)|^2 + |\psi_B(x_1)|^2 |\psi_A(x_2)|^2) - \\
&\quad \frac{1}{2} (\psi_A^*(x_1) \psi_B^*(x_2) \psi_B(x_1) \psi_A(x_2) + \psi_B^*(x_1) \psi_A^*(x_2) \psi_A(x_1) \psi_B(x_2)),
\end{aligned}$$

which contains two contributions

$$p(x_1, x_2) = p_{\text{cl}}(x_1, x_2) - p_{\text{qu}}(x_1, x_2), \quad (426)$$

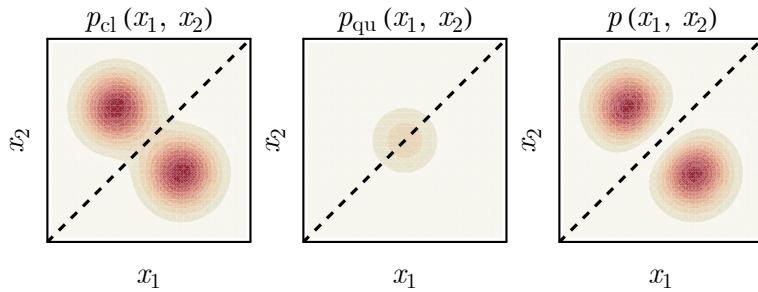
- the **classical part** is just the symmetrized product distribution

$$p_{\text{cl}}(x_1, x_2) = \frac{1}{2} (p_A(x_1) p_B(x_2) + p_B(x_1) p_A(x_2)), \quad (427)$$

where $p_{A/B}(x) = |\psi_{A/B}(x)|^2$.

- the **quantum part** is a correction that originates from *quantum interference* between fermions

$$p_{\text{qu}}(x_1, x_2) = \frac{1}{2} (\psi_A^*(x_1) \psi_B^*(x_2) \psi_B(x_1) \psi_A(x_2) + \psi_B^*(x_1) \psi_A^*(x_2) \psi_A(x_1) \psi_B(x_2)). \quad (428)$$



- The average **interaction energy**

$$E_U = \int dx_1 dx_2 U(x_1 - x_2) p(x_1, x_2) \quad (429)$$

will also contain two terms

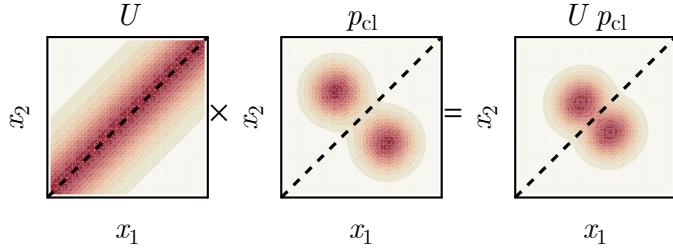
$$E_U = E_{\text{Hart}} - E_{\text{Fock}}, \quad (430)$$

- the **Hartree energy** (direct energy) from the classical contribution

$$\begin{aligned}
E_{\text{Hart}} &= \int dx_1 dx_2 U(x_1 - x_2) p_{\text{cl}}(x_1, x_2) \\
&= \int dx_1 dx_2 U(x_1 - x_2) |\psi_A(x_1)|^2 |\psi_B(x_2)|^2.
\end{aligned} \quad (431)$$

In terms of the Dirac notation

$$E_{\text{Hart}} = \langle \psi_A \psi_B | U | \psi_A \psi_B \rangle. \quad (432)$$

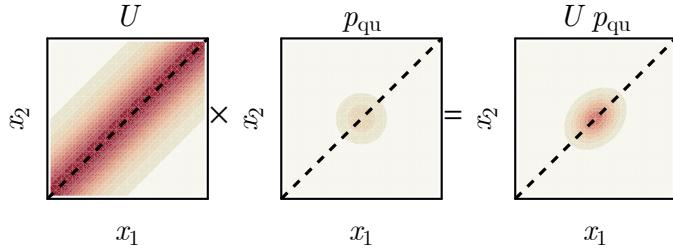


- the **Fock energy** (exchange energy) from the quantum correction

$$\begin{aligned} E_{\text{Fock}} &= \int dx_1 dx_2 U(x_1 - x_2) p_{\text{qu}}(x_1, x_2) \\ &= \int dx_1 dx_2 U(x_1 - x_2) \psi_A^*(x_1) \psi_B^*(x_2) \psi_B(x_1) \psi_A(x_2). \end{aligned} \quad (433)$$

In terms of the Dirac notation

$$E_{\text{Fock}} = \langle \psi_A \psi_B | U | \psi_B \psi_A \rangle. \quad (434)$$



■ Hartree-Fock Approximation

Hartree-Fock approximation is a *variational approach* to solve for the ground state of interacting fermion systems.

$$H = \sum_i \underbrace{\frac{\mathbf{p}_i^2}{2m} + V(\mathbf{x}_i)}_{H_0} + \sum_{i \neq j} U(\mathbf{x}_i - \mathbf{x}_j). \quad (435)$$

- It assumes that the N -body ground state can be *approximated* by the state of N fermions separately occupying N single-particle orbitals.
- By optimizing the orbital wave functions to minimize the energy, one can estimate the ground state energy as well as the approximate ground state wave function.

For example, consider a two-body system ($N = 2$) in 1D

$$H = H_0(p_1, x_1) + H_0(p_2, x_2) + U(x_1 - x_2) \quad (436)$$

Two orthonormal orbitals will be introduced, denoted as $\psi_A(x)$ and $\psi_B(x)$, and the variational state is taken to be

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} (\psi_A(x_1) \psi_B(x_2) - \psi_B(x_1) \psi_A(x_2)). \quad (437)$$

The energy expectation value is given by

$$\langle \psi | H | \psi \rangle = \langle \psi_A | H_0 | \psi_A \rangle + \langle \psi_B | H_0 | \psi_B \rangle + \underbrace{\langle \psi_A \psi_B | U | \psi_A \psi_B \rangle}_{\text{Hartree}} - \underbrace{\langle \psi_A \psi_B | U | \psi_B \psi_A \rangle}_{\text{Fock}}. \quad (438)$$

where

- the A orbital energy is (similar for B orbital)

$$\langle \psi_A | H_0 | \psi_A \rangle = \int dx \psi_A^*(x) \left(-\frac{\hbar^2}{2m} \partial_x^2 + V(x) \right) \psi_A(x). \quad (439)$$

- the Hartree energy

$$\langle \psi_A \psi_B | U | \psi_A \psi_B \rangle = \int dx_1 dx_2 U(x_1 - x_2) |\psi_A(x_1)|^2 |\psi_B(x_2)|^2, \quad (440)$$

- the Fock energy

$$\langle \psi_A \psi_B | U | \psi_B \psi_A \rangle = \int dx_1 dx_2 U(x_1 - x_2) \psi_A^*(x_1) \psi_B^*(x_2) \psi_B(x_1) \psi_A(x_2). \quad (441)$$

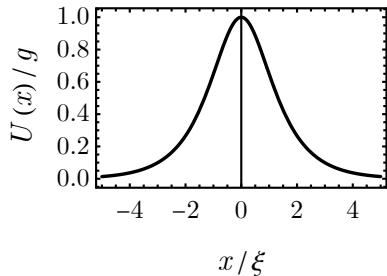
Objective: optimize the functions $\psi_A(x)$ and $\psi_B(x)$ to minimize $\langle \psi | H | \psi \rangle$.

- The minimal value of $\langle \psi | H | \psi \rangle$ provides an estimation of the ground state energy.
- The optimal orbitals can be used to construct the many-body state $\psi(x_1, x_2)$, which is a variational approximation of the ground state.

□ Two Electrons in a Box

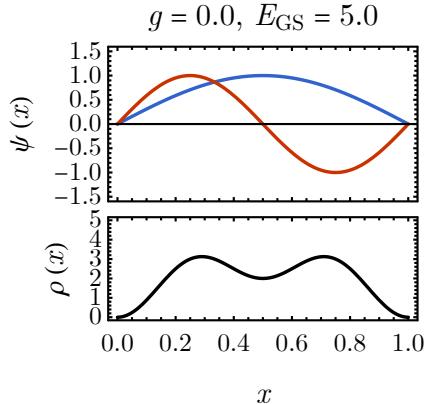
Consider two (spinless) electrons confined in a 1D box (infinite square potential $x \in [0, 1]$) interacting with each other via an repulsive potential

$$U(x) = g \operatorname{sech}\left(\frac{x}{\xi}\right), \quad (442)$$

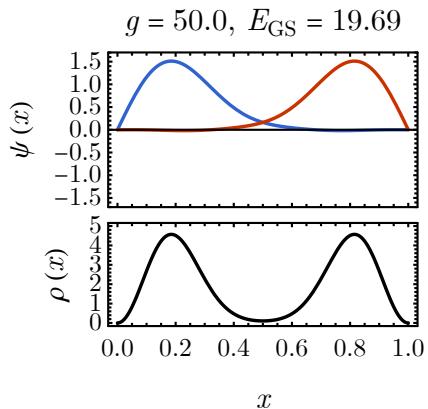


- Non-interacting limit ($g = 0$): the electrons will occupy the lowest two orbitals in the square well. The single-electron density distribution can be calculated from

$$\rho(x) = \int |\psi(x, x')|^2 dx' = |\psi_A(x)|^2 + |\psi_B(x)|^2. \quad (443)$$



- The electrons are repelled from the infinite walls \Rightarrow density vanishes approaching both walls.
- The electrons do not want to stay with each other (Pauli exclusion) \Rightarrow a small dip in the middle part of the density distribution.
- Strong-interacting limit ($g \rightarrow \infty$): the electrons will further repel each other \Rightarrow a deeper suppression of density in the middle, breaking the distribution into two peaks.



- Two *localized* orbitals emerge. Each electron occupies one localized orbital, and does not want to travel to the other side of the box.
- For more electrons (and in higher dimensions), this will lead to crystallization of electrons \Rightarrow **Wigner crystal**.

■ Quantum Origin of Magnetism

■ Exchange Interaction (Ferromagnetism)

The above discussion has not included the internal spin state of the electron. The many-body state of electrons must be *totally* antisymmetric upon exchanging electrons in the *orbital* and the *spin* Hilbert spaces jointly: if the spin state is already symmetric/antisymmetric, the orbital state must be antisymmetric/symmetric.

For two electrons, each carries spin-1/2 (two states $|\uparrow\rangle$ and $|\downarrow\rangle$)

- Antisymmetric spin state \rightarrow **spin singlet** state ($s = 0$)

$$\begin{array}{ccc} s & m_s \\ 0 & 0 & \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \end{array} \quad (444)$$

Spins are anti-aligned as $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = -3 \hbar^2 / 4 < 0 \Rightarrow$ **antiferromagnetic**.

- Symmetric spin states \rightarrow **spin triplet** states ($s = 1$)

$$\begin{array}{ccc} s & m_s \\ 1 & +1 & |\uparrow\uparrow\rangle \\ 1 & 0 & \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ 1 & -1 & |\downarrow\downarrow\rangle \end{array} \quad (445)$$

Spins are aligned as $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = \hbar^2 / 4 > 0 \Rightarrow$ **ferromagnetic**.

Suppose there are two energetically-degenerated orbitals $\psi_A(x)$ and $\psi_B(x)$ to occupied, the electrons can be either of the following states:

- Orbital symmetric, Spin antisymmetric (antiferromagnetic)

$$\frac{1}{\sqrt{2}} (\langle \psi_A | \psi_B \rangle + \langle \psi_B | \psi_A \rangle) \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad (446)$$

\rightarrow Interaction energy

$$E_U = \langle \psi_A | \psi_B | U | \psi_A | \psi_B \rangle + \langle \psi_A | \psi_B | U | \psi_B | \psi_A \rangle. \quad (447)$$

- Orbital antisymmetric, Spin symmetric (ferromagnetic)

$$\frac{1}{\sqrt{2}} (\langle \psi_A | \psi_B \rangle - \langle \psi_B | \psi_A \rangle) \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \quad (448)$$

\rightarrow Interaction energy

$$E_U = \langle \psi_A | \psi_B | U | \psi_A | \psi_B \rangle - \langle \psi_A | \psi_B | U | \psi_B | \psi_A \rangle. \quad (449)$$

Assuming the Fock energy is positive $\langle \psi_A | \psi_B | U | \psi_B | \psi_A \rangle > 0$ (e.g. the repulsive Coulomb interaction), then the ferromagnetic state is lower in energy.

- **Spin exchange interaction:** the ferromagnetic spin-spin interaction between two electrons occupying two degenerated orbitals.

- This *magnetic* (spin) interaction originates from the *quantum* effect of the *electric* (charge) interaction (the exchange energy of Coulomb interaction). The fermionic nature of electron plays a key role in this mechanism.

[If the spin interaction was originated from the magnetic dipole interaction (electromagnetic force), the spins should tend to anti-align with each other, which makes it hard to explain the existence of ferromagnets.]

- **Hund's rule:** atomic orbitals in the same energy shell tend to be singly occupied by electrons of the same spin (to maximize the total spin).

This is a result of the spin exchange interaction between electrons on these orbitals.

- **Magnetic interaction in molecules and solids.** The spin exchange interaction is less effective between electrons from different atoms, because the overlap $\langle \psi_A | \psi_B \rangle$ between orbital wave functions is small, and the exchange interaction is also small in general. There is a competing effect in this case: both electrons tends to occupy the *bonding orbital* $|\psi_A\rangle + |\psi_B\rangle$ to lower the *kinetic* energy, then the spin must be anti-aligned due to the Pauli exclusion principle → leading to the *antiferromagnetic* interaction between electrons in a covalent bond.

mechanism	type	origin
covalent bond	antiferro	kinetic energy
spin exchange	ferro	interaction energy

It is quit subtle to determine whether electron spins on neighboring atoms want to be aligned or anti-aligned. Generally either behavior is possible.

■ Super-Exchange Interaction (Antiferromagnetism)

Hubbard model: tight binding model + on-site interaction (Hubbard interaction). It provides a good explanation for the *antiferromagnetic* interaction between electrons from neighboring atoms.

- Consider two sites (atoms) A and B adjacent to each other, with a total of two electrons.

- For each electron, there are *four* possible states

$$|A_{\uparrow}\rangle, |A_{\downarrow}\rangle, |B_{\uparrow}\rangle, |B_{\downarrow}\rangle. \quad (450)$$

- Two electrons together has *six* possible states ($C_4^2 = 6$)

$$\begin{aligned} |A_{\uparrow} B_{\uparrow}\rangle &= -|B_{\uparrow} A_{\uparrow}\rangle, \\ |A_{\uparrow} B_{\downarrow}\rangle &= -|B_{\downarrow} A_{\uparrow}\rangle, \\ |A_{\downarrow} B_{\uparrow}\rangle &= -|B_{\uparrow} A_{\downarrow}\rangle, \\ |A_{\downarrow} B_{\downarrow}\rangle &= -|B_{\downarrow} A_{\downarrow}\rangle, \\ |A_{\uparrow} A_{\downarrow}\rangle &= -|A_{\downarrow} A_{\uparrow}\rangle, \\ |B_{\uparrow} B_{\downarrow}\rangle &= -|B_{\downarrow} B_{\uparrow}\rangle. \end{aligned} \quad (451)$$

- Hopping term H_{hop} turns a A_{\uparrow} orbital to a B_{\uparrow} orbital and vice versa, and similarly turns a A_{\downarrow} orbital to a B_{\downarrow} orbital and vice versa (electron hopping is independent of spin).

- For example, starting from $|A_{\uparrow} B_{\downarrow}\rangle$,

$$\langle A_{\uparrow} A_{\downarrow} | H_{\text{hop}} | A_{\uparrow} B_{\downarrow} \rangle = -t, \quad (452)$$

$$\langle B_{\uparrow} B_{\downarrow} | H_{\text{hop}} | A_{\uparrow} B_{\downarrow} \rangle = -t;$$

starting from $|A_{\downarrow} B_{\uparrow}\rangle$,

$$\begin{aligned}\langle A_\downarrow A_\uparrow | H_{\text{hop}} | A_\downarrow B_\uparrow \rangle &= -t, \\ \langle B_\downarrow B_\uparrow | H_{\text{hop}} | A_\downarrow B_\uparrow \rangle &= -t,\end{aligned}\quad (453)$$

which can also be written as

$$\begin{aligned}\langle A_\uparrow A_\downarrow | H_{\text{hop}} | A_\downarrow B_\uparrow \rangle &= t, \\ \langle B_\uparrow B_\downarrow | H_{\text{hop}} | A_\downarrow B_\uparrow \rangle &= t,\end{aligned}\quad (454)$$

given the basis relations in Eq. (451).

- If the electron spins are *aligned*, *no hopping* can occur. As hopping processes like

$$\begin{aligned}|A_\uparrow B_\uparrow\rangle \rightarrow |B_\uparrow B_\uparrow\rangle &= 0, \\ |A_\uparrow B_\uparrow\rangle \rightarrow |A_\uparrow A_\uparrow\rangle &= 0,\end{aligned}\quad (455)$$

are forbidden by the *Pauli exclusion* principle.

- The hopping Hamiltonian can be represented as a matrix

$$H_{\text{hop}} \simeq \left(\begin{array}{cccc|cc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -t & -t \\ 0 & 0 & 0 & 0 & t & t \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & -t & t & 0 & 0 & 0 \\ 0 & -t & t & 0 & 0 & 0 \end{array} \right). \quad (456)$$

- Interaction term H_{int} gives energy penalty $U > 0$ when two electrons are on the same site (such that they repel strongly)

$$\begin{aligned}\langle A_\uparrow A_\downarrow | H_{\text{int}} | A_\uparrow A_\downarrow \rangle &= U, \\ \langle B_\uparrow B_\downarrow | H_{\text{int}} | B_\uparrow B_\downarrow \rangle &= U,\end{aligned}\quad (457)$$

which can be represented as a diagonal matrix for the last two states

$$H_{\text{int}} \simeq \left(\begin{array}{cccc|cc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & U & 0 \\ 0 & 0 & 0 & 0 & 0 & U \end{array} \right). \quad (458)$$

Put together the two-site Hubbard model Hamiltonian $H = H_{\text{hop}} + H_{\text{int}}$ can be written as

$$H \simeq \left(\begin{array}{cccc|cc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -t & -t \\ 0 & 0 & 0 & 0 & t & t \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & -t & t & 0 & U & 0 \\ 0 & -t & t & 0 & 0 & U \end{array} \right). \quad (459)$$

- The *spin-triplet* states are eigenstates of H of the eigen energy $E = 0$

energy	state
0	$ A_\uparrow B_\uparrow\rangle$
0	$\frac{1}{\sqrt{2}} (A_\uparrow B_\downarrow\rangle + A_\downarrow B_\uparrow\rangle)$
0	$ A_\downarrow B_\downarrow\rangle$

(460)

- The following double occupied (anti-bonding) state is “dark” to hopping, which is also an eigen-state of H of energy $E = U$,

energy	state
U	$\frac{1}{\sqrt{2}} (A_\uparrow A_\downarrow\rangle - B_\uparrow B_\downarrow\rangle)$

(461)

- The *spin-singlet* state and the *double occupied* (bonding) states can turn into each other via hopping,

$$\begin{aligned} |s\rangle &= \frac{1}{\sqrt{2}} (|A_\uparrow B_\downarrow\rangle - |A_\downarrow B_\uparrow\rangle), \\ |d\rangle &= \frac{1}{\sqrt{2}} (|A_\uparrow A_\downarrow\rangle + |B_\uparrow B_\downarrow\rangle). \end{aligned} \quad (462)$$

The Hamiltonian projected to the $|s\rangle, |d\rangle$ basis will be represented as

$$H \approx \begin{pmatrix} 0 & -2t \\ -2t & U \end{pmatrix}. \quad (463)$$

- Strong interaction limit $U \gg t$, the ground state $|s\rangle + O(t/U)$ is very close to the spin-singlet state $|s\rangle$ with the eigen energy

$$E = -\frac{4t^2}{U}, \quad (464)$$

which is also the energy splitting between singlet and triplet state. In a spin model $H = J \mathbf{S}_1 \cdot \mathbf{S}_2$, the energy splitting between the singlet ($E = -3J/4$) and triplet ($E = J/4$) states is simply J .

Therefore Eq. (464) implies that the electronic system can be effectively viewed as a spin system in the strong interaction regime with an *antiferromagnetic* spin coupling

$$J = \frac{4t^2}{U}, \quad (465)$$

which is also known as the **super-exchange interaction**.

- Weak interaction limit $U \ll t$, the ground state is

$$\frac{1}{\sqrt{2}} (|s\rangle + |d\rangle)$$

$$\begin{aligned}
&= \frac{1}{2} (|A_\uparrow A_\downarrow\rangle + |A_\uparrow B_\downarrow\rangle - |A_\downarrow B_\uparrow\rangle + |B_\uparrow B_\downarrow\rangle) \\
&= \frac{1}{2} (|A_\uparrow A_\downarrow\rangle + |A_\uparrow B_\downarrow\rangle + |B_\downarrow A_\uparrow\rangle + |B_\uparrow B_\downarrow\rangle) \\
&= \frac{1}{\sqrt{2}} (|A_\uparrow\rangle + |B_\uparrow\rangle) \otimes \frac{1}{\sqrt{2}} (|A_\downarrow\rangle + |B_\downarrow\rangle),
\end{aligned}$$

with eigen energy $-2t$. This describes two electrons with opposite spins occupying the single-particle bonding state together. Each electron gains the energy t as the kinetic energy is reduced by hybridizing the two atomic orbitals.

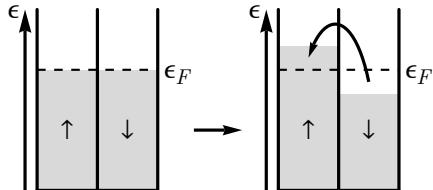
- In both limits, the ground state is a spin-singlet state (antiferromagnetic). As the interaction is turned on it simply suppresses the component of the double occupied state $|d\rangle$ in the ground state.

■ Instabilities of Metallic State

■ Itinerant Ferromagnetism

For free electron system, it is always energetically favorable to have the same number of up and down spins ($N_\uparrow = N_\downarrow$), than to have the number differ.

- Because creating the *spin imbalance* (say $N_\uparrow > N_\downarrow$) corresponds to transferring some of the \downarrow spin electrons from below the Fermi energy to \uparrow spin electrons above the Fermi energy, which will always *increase* the energy.



- This can also be seen from the *positive* spin susceptibility χ of electron gas calculated in Eq. (376),

$$\chi = \frac{\partial M}{\partial B} = \mu_B^2 \frac{2 g(\epsilon_F)}{n}, \quad (467)$$

meaning that the total energy E_0 of a free electron system must grow with the magnetization M as

$$\frac{E_0}{N} = \frac{1}{2\chi} M^2 - M B, \quad (468)$$

such that the minimal energy solution is always given by $M = \chi B$ (matching the paramagnetic behavior characterized by χ).

This would predict that metals do not want to spontaneously magnetize in the absence of mag-

netic field. But how to explain the existence of ferromagnetic metals, like iron (Fe), nickel (Ni), cobalt (Co) etc.?

Electron interaction plays a central role in explaining the magnetism in materials.

- Consider a short-range interaction between electrons modeled by an interaction potential

$$U(\mathbf{x} - \mathbf{x}') = U_0 \delta(\mathbf{x} - \mathbf{x}'). \quad (469)$$

Electron repels (assuming $g > 0$) each other when they are in contact at a point. This mimics the behavior of (screened) Coulomb interaction.

- For electrons of the same spin,

- the Hartree energy

$$\begin{aligned} E_{\text{Hartree}} &= \sum_{\epsilon_k, \epsilon_{k'} < \mu_\uparrow} \langle \psi_{k\uparrow} \psi_{k'\uparrow} | U | \psi_{k\uparrow} \psi_{k'\uparrow} \rangle \\ &= U_0 \sum_{\epsilon_k, \epsilon_{k'} < \mu_\uparrow} \int d\mathbf{x}_1 d\mathbf{x}_2 \delta(\mathbf{x}_1 - \mathbf{x}_2) |\psi_k(\mathbf{x}_1)|^2 |\psi_{k'}(\mathbf{x}_2)|^2 \\ &= U_0 \sum_{\epsilon_k, \epsilon_{k'} < \mu_\uparrow} \int d\mathbf{x} |\psi_k(\mathbf{x})|^2 |\psi_{k'}(\mathbf{x})|^2 \\ &= U_0 \sum_{\epsilon_k, \epsilon_{k'} < \mu_\uparrow} \frac{1}{V} \\ &= \frac{U_0 N_\uparrow^2}{V}, \end{aligned} \quad (470)$$

- the Fock energy is

$$\begin{aligned} E_{\text{Fock}} &= \sum_{\epsilon_k, \epsilon_{k'} < \mu_\uparrow} \langle \psi_{k\uparrow} \psi_{k'\uparrow} | U | \psi_{k'\uparrow} \psi_{k\uparrow} \rangle \\ &= U_0 \sum_{\epsilon_k, \epsilon_{k'} < \mu_\uparrow} \int d\mathbf{x}_1 d\mathbf{x}_2 \delta(\mathbf{x}_1 - \mathbf{x}_2) \psi_k^*(\mathbf{x}_1) \psi_{k'}^*(\mathbf{x}_2) \psi_{k'}(\mathbf{x}_1) \psi_k(\mathbf{x}_2) \\ &= U_0 \sum_{\epsilon_k, \epsilon_{k'} < \mu_\uparrow} \int d\mathbf{x} |\psi_k(\mathbf{x})|^2 |\psi_{k'}(\mathbf{x})|^2 \\ &= U_0 \sum_{\epsilon_k, \epsilon_{k'} < \mu_\uparrow} \frac{1}{V} \\ &= \frac{U_0 N_\uparrow^2}{V}, \end{aligned} \quad (471)$$

- the Hartree energy is precisely canceled by the Fock energy, and the total interaction energy *vanishes* for same-spin electrons under *short-range* interaction,

$$E_U = E_{\text{Hartree}} - E_{\text{Fock}} = 0. \quad (472)$$

This can be understood as a consequence of the *Pauli exclusion principle* that forbids the

same-spin electrons to come to the same point to interact.

- For electrons of opposite spins,

- the Hartree energy is similar

$$\begin{aligned}
 E_{\text{Hartree}} &= \sum_{\epsilon_k < \mu_\uparrow} \sum_{\epsilon_{k'} < \mu_\downarrow} \langle \psi_{k\uparrow} \psi_{k'\downarrow} | U | \psi_{k\uparrow} \psi_{k'\downarrow} \rangle \\
 &= U_0 \sum_{\epsilon_k < \mu_\uparrow} \sum_{\epsilon_{k'} < \mu_\downarrow} \int d\mathbf{x}_1 d\mathbf{x}_2 \delta(\mathbf{x}_1 - \mathbf{x}_2) |\psi_{\mathbf{k}}(\mathbf{x}_1)|^2 |\psi_{\mathbf{k}'}(\mathbf{x}_2)|^2 \\
 &= U_0 \sum_{\epsilon_k < \mu_\uparrow} \sum_{\epsilon_{k'} < \mu_\downarrow} \int d\mathbf{x} |\psi_{\mathbf{k}}(\mathbf{x})|^2 |\psi_{\mathbf{k}'}(\mathbf{x})|^2 \\
 &= U_0 \sum_{\epsilon_k < \mu_\uparrow} \sum_{\epsilon_{k'} < \mu_\downarrow} \frac{1}{V} \\
 &= \frac{U_0 N_\uparrow N_\downarrow}{V}.
 \end{aligned} \tag{473}$$

- But there is no Fock energy contribution, because the orbital state can either be symmetric or antisymmetric (as the spin state can adjust accordingly), the two possibilities have opposite signs in front of their Fock energies, which cancel out.
- So the total interaction energy for opposite-spin electrons is

$$E_U = E_{\text{Hartree}} = \frac{U_0 N_\uparrow N_\downarrow}{V}. \tag{474}$$

Put together, the interaction energy of the electronic system is

$$\begin{aligned}
 E_U &= \frac{U_0 N_\uparrow N_\downarrow}{V} \\
 &= \frac{U_0}{4V} ((N_\uparrow + N_\downarrow)^2 - (N_\uparrow - N_\downarrow)^2) \\
 &= \frac{U_0 N^2}{4V} \left(1 - \left(\frac{M}{\mu_B}\right)^2\right).
 \end{aligned} \tag{475}$$

- $N = N_\uparrow + N_\downarrow$: total number of electrons,

- $M = \mu_B \frac{N_\uparrow - N_\downarrow}{N}$: magnetization, average magnetic moment per electron.

The total energy $E = E_0 + E_U$ of the system sums up contributions from both the kinetic (band) energy E_0 and the interaction energy E_U

$$\begin{aligned}
 \frac{E_0 + E_U}{N} &= \frac{1}{2\chi} M^2 - \frac{U_0 n}{4\mu_B^2} M^2 + \text{const} \\
 &= \frac{n}{4\mu_B^2} \left(\frac{1}{g(\epsilon_F)} - U_0 \right) M^2 + \text{const}
 \end{aligned} \tag{476}$$

The stability of the system relies on the sign of the quadratic coefficient in front of M^2 .

- When $g(\epsilon_F)^{-1} - U_0 > 0$, the energy minimum is at zero magnetization $M = 0$. \Rightarrow The electronic system is **stable** in the spin-balanced state \Rightarrow **paramagnetic metal**.
- When $g(\epsilon_F)^{-1} - U_0 < 0$, the system can lower its energy by keep increasing the magnetization M (until some higher-order effects set in to determine the saturation value of M). \Rightarrow The spin-balanced electronic system is **unstable** towards spontaneous magnetization \Rightarrow **ferromagnetic metal**.

Stoner Criterion: the condition for itinerant ferromagnetism to develop in electronic systems is

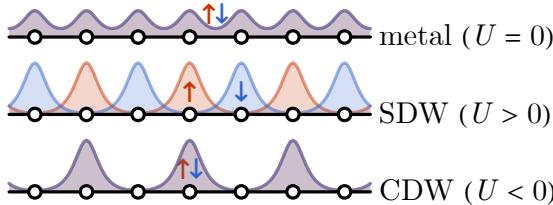
$$U_0 g(\epsilon_F) > 1, \quad (477)$$

i.e. the interaction must be repulsive and must be strong enough to overcome the kinetic energy loss.

■ Spin/Charge Density Wave

In the lattice system, electron interactions can lead to formation of density waves. Consider spin-1/2 electrons hopping on a 1D lattice, with on-site *Hubbard interaction*

$$\begin{aligned} H &= H_0 + H_{\text{int}}, \\ H_0 &= -t \sum_i \sum_{\sigma=\uparrow,\downarrow} (c_{i+1\sigma}^\dagger c_{i\sigma} + \text{h.c.}), \\ H_{\text{int}} &= U \sum_i n_{i\uparrow} n_{i\downarrow}. \end{aligned} \quad (478)$$



- At *half filling*, on average there is *one* electron per site (a site can at most host two electrons of \uparrow and \downarrow spins). Without interaction, the system is in the *metallic* phase.
- When $U > 0$ (*repulsive* interaction), \uparrow and \downarrow spin electrons do not want to stay on the same site to avoid repulsive interaction \Rightarrow different spins will spontaneously occupy alternative sites \Rightarrow **spin density wave (SDW)**.
- When $U < 0$ (*attractive* interaction), \uparrow and \downarrow spin electrons wants to stay on the same site to gain attractive interaction \Rightarrow electrons will spontaneously doubly occupy half of the sites and empty the other half alternatively \Rightarrow **charge density wave (CDW)**.
- Both SDW/CDW order *spontaneously* breaks the **lattice translation symmetry** and *doubles* the primitive unit cell.

To model the density wave state, consider a variational state as the ground state of a mean-field Hamiltonian

$$H_{\text{MF}} = -\frac{u}{2} \sum_i (|i+1\rangle\langle i| + \text{h.c.}) - v \sum_i (-1)^i |i\rangle\langle i|. \quad (479)$$

- u - hopping strength of the mean-field model, set to $u = 1$ in the end (H_{MF} can always be rescaled by an overall factor without affecting the variational ground state).
- v - stagger potential, serves as the *variational parameter*, controls the *ordering strength*.

Take the two-site unit-cell, transform to the momentum space

$$\begin{aligned} |k, A\rangle &= L^{-1/2} \sum_{i \in A} e^{ikx_i} |i\rangle, \\ |k, B\rangle &= L^{-1/2} \sum_{i \in B} e^{ikx_i} |i\rangle, \end{aligned} \quad (480)$$

- A sublattice: i is even, B sublattice: i is odd.
- L - number of unit cell (not using N to avoid confusion with the total electron number).
- Site coordinate $x_i = i$ (unit cell volume = 2).
- First Brillouin zone: $k \in [-\pi/2, \pi/2]$.

Focus on one spin species, the mean-field Hamiltonian reads

$$H_{\text{MF}} = - \sum_k (u \cos k |k, A\rangle\langle k, B| + \text{h.c.}) - v \sum_k (|k, A\rangle\langle k, A| - |k, B\rangle\langle k, B|), \quad (481)$$

or in matrix representation as

$$H \simeq \bigoplus_k H_k, \quad H_k \simeq - \begin{pmatrix} v & u \cos k \\ u \cos k & -v \end{pmatrix} \quad (482)$$

- Band dispersion

$$\epsilon_{k,\pm} = \pm \sqrt{(u \cos k)^2 + v^2} \quad (483)$$

The stagger potential v opens a gap, splitting spectrum into two bands. Half-filling the electronic system \Rightarrow fully occupies the lower band.

Total mean-field energy for the spin species (at $T = 0$)

$$\begin{aligned} \langle H_{\text{MF}} \rangle &= \sum_{k \in \text{BZ}} \epsilon_{k,-} = - \sum_{k \in \text{BZ}} \sqrt{(u \cos k)^2 + v^2} \\ &= -L \int_{-\pi/2}^{\pi/2} \frac{dk}{\pi} \sqrt{(u \cos k)^2 + v^2}. \end{aligned} \quad (484)$$

- Define the expected bonding strength (for single spin species)

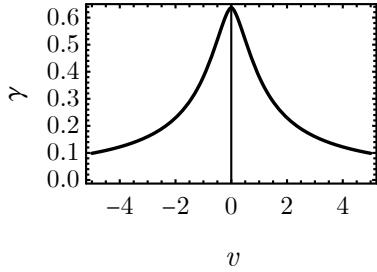
$$\gamma = 2 \langle c_{i+1}^\dagger c_i + \text{h.c.} \rangle, \quad (485)$$

It can be evaluated from

$$\left\langle \frac{\partial H_{\text{MF}}}{\partial u} \right\rangle_{u=1} = -L \gamma, \quad (486)$$

therefore

$$\gamma = \int_{-\pi/2}^{\pi/2} \frac{dk}{\pi} \frac{\cos^2 k}{\sqrt{\cos^2 k + v^2}}. \quad (487)$$



- Define the expected density imbalance (for single spin species)

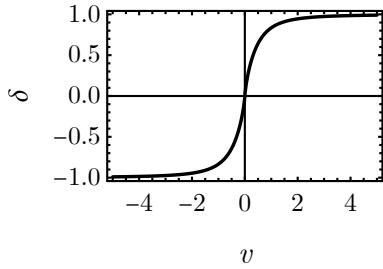
$$\delta = \langle n_A \rangle - \langle n_B \rangle. \quad (488)$$

It can be evaluated from

$$\left\langle \frac{\partial H_{\text{MF}}}{\partial v} \right\rangle_{u=1} = -L\delta, \quad (489)$$

therefore

$$\delta = \int_{-\pi/2}^{\pi/2} \frac{dk}{\pi} \frac{v}{\sqrt{\cos^2 k + v^2}}. \quad (490)$$



Given that $\langle n_A \rangle + \langle n_B \rangle = 1$ (filling one band \Leftrightarrow one fermion per unit cell),

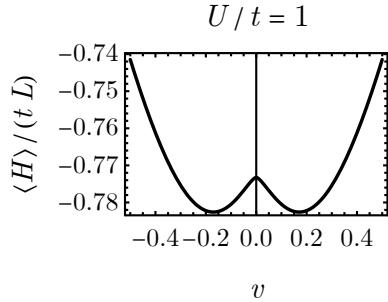
$$\langle n_A \rangle = \frac{1+\delta}{2}, \langle n_B \rangle = \frac{1-\delta}{2}. \quad (491)$$

With these preparations,

- The expectation energy for the SDW state is

$$\begin{aligned} \frac{\langle H \rangle}{L} &= -2t\gamma + U(2\langle n_A \rangle \langle n_B \rangle) \\ &= -2t\gamma + \frac{U}{2}(1 - \delta^2), \end{aligned} \quad (492)$$

which has non-trivial minimum at $v \neq 0$ when $U > 0$.



- The energy minimum is achieved at $\partial_v \langle H \rangle = 0$ (excluding the $v = 0$ solution), which is given by the **mean-field equation**

$$1 - \frac{U}{2 t} \int_{-\pi/2}^{\pi/2} \frac{dk}{\pi} \frac{1}{\sqrt{\cos^2 k + v^2}} = 0. \quad (493)$$

**Exc
16**

Derive Eq. (493).

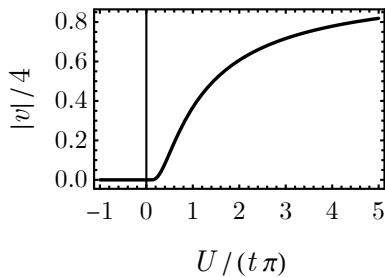
- For small U/t (hence small v) the equation can be approximated by

$$1 - \frac{U}{2 t} \frac{2}{\pi} \ln\left(\frac{4}{|v|}\right) = 0, \quad (500)$$

whose solution is

$$|v| = 4 \exp\left(-\frac{t \pi}{U}\right). \quad (501)$$

The **SDW gap** $|v|$ opens with the repulsive interaction U non-perturbatively.



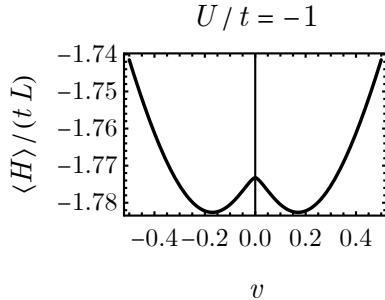
- Correspondingly, the **SDW order parameter** δ is also induced non-perturbatively

$$|\delta| = \frac{t}{2 U} \exp\left(-\frac{t \pi}{U}\right). \quad (502)$$

- The expectation energy for the CDW state is

$$\begin{aligned} \frac{\langle H \rangle}{L} &= -2 t \gamma + U (\langle n_A \rangle^2 + \langle n_B \rangle^2) \\ &= -2 t \gamma + \frac{U}{2} (1 + \delta^2), \end{aligned} \quad (503)$$

which has non-trivial minimum at $v \neq 0$ when $U < 0$.



The energy minimum is achieved at $\partial_v \langle H \rangle = 0$ (excluding the $v = 0$ solution), which is given by the **mean-field equation**

$$1 - \frac{(-U)}{2t} \int_{-\pi/2}^{\pi/2} \frac{dk}{\pi} \frac{1}{\sqrt{\cos^2 k + v^2}} = 0. \quad (504)$$

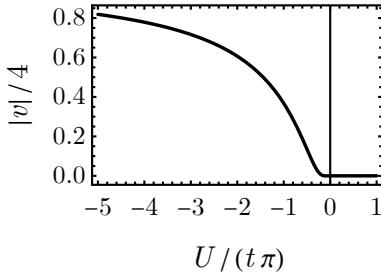
- For small U/t (hence small v) the equation can be approximated by

$$1 - \frac{(-U)}{2t} \frac{2}{\pi} \ln\left(\frac{4}{|v|}\right) = 0, \quad (505)$$

whose solution is

$$|v| = 4 \exp\left(-\frac{t\pi}{(-U)}\right). \quad (506)$$

The **CDW gap** $|v|$ opens with the attractive interaction $(-U)$ non-perturbatively.



- Correspondingly, the **CDW order parameter** δ is also induced non-perturbatively.

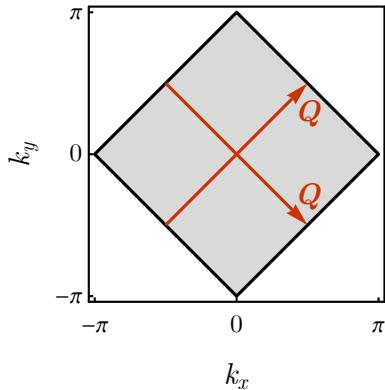
$$|\delta| = \frac{t}{2(-U)} \exp\left(-\frac{t\pi}{(-U)}\right). \quad (507)$$

In conclusion, the 1D (half-filled) metallic state is *unstable* under interaction. Infinitesimal interaction (no matter repulsive or attractive) will trigger the development of **density wave order** that

spontaneously breaks the **lattice translation symmetry**. Its consequence can be observed by scattering experiments, that new satellite peaks will appear due to the scattering with spin/charge modulations.

The same phenomenon also happens in higher dimension, when the Fermi surface is *nested*.

- For example, half-filled square lattice hopping model has a square-shaped Fermi surface, where parallel edges *coincide* when shifted by the **nesting momentum** \mathbf{Q} .



- The phenomenon of two finite segments of the Fermi surface are connected by the same moment shift is called **Fermi surface nesting**. In this case, the Fermi surface has an instability towards SDW/CDW ordering under interaction. The **density wave vector** is set by the **nesting momentum**.
- Density wave order generally leads to **gap opening** on the Fermi surface. At the low temperature limit ($T = 0$), the gap size Δ scales with interaction strength U as

$$\Delta \sim \exp\left(-\frac{1}{2 U g(\epsilon_F)}\right), \quad (508)$$

where $g(\epsilon_F)$ is the Fermi surface density of state.