Quantum Transport Theory

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Victory won't come to us unless we go to it.

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Chapter 1 Introduction

1.1 Classic Transport Theory: Drude-Boltzmann Method

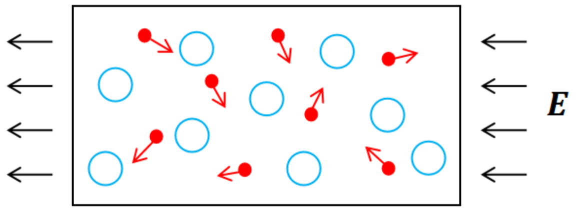
The Drude model is proposed by Paul Drude in 1900, before the clear understanding of the structure of atoms. It assumes electrons transport in the metal undergoing random scattering. The basic assumptions include

(1) Electrons transport freely between collisions.

(2) Collisions are instantaneous events.

(3) **Mean free time** between collisions is τ_c, which is independent of position and velocity. τ_m is the momentum relaxation time.

(4) Electrons achieve local thermal equilibrium.



Given the momentum $p(t)$ of an electron e at time t. During $t \to t + dt$, e may move freely with the probability $1 - dt/\tau_m$ and gain addition momentum $f(t)dt$, where f is the external force. It may undergo collision with the probability dt/τ_m and lose all information of its momentum and gain a momentum $f(t)dt$. Thus the momentum at $t + dt$ is

$$p(t + dt) = (1 - \frac{dt}{\tau_m})[p(t) + f(t)dt] + \frac{p_{ran}dt}{\tau_m} + f(t)dt \cdot \frac{dt}{\tau_m} \tag{1.1}$$

where $p_{ran}dt/\tau_m$ is the dissipation term. By taking the average, one obtains

$$\overline{p}(t + dt) - \overline{p}(t) = -\frac{dt}{\tau_m}\overline{p}(t) + \overline{f}(t)dt + \overline{p}_{ran}\frac{dt}{\tau_m} \tag{1.2}$$

By using $\overline{p}_{ran} = 0$,

$$\begin{aligned} \overline{p}(t + dt) - \overline{p}(t) &= -\frac{dt}{\tau_m}\overline{p}(t) + \overline{f}(t)dt \\ \frac{d\overline{p}(t)}{dt} &= \overline{f}(t) - \frac{\overline{p}(t)}{\tau_m} \end{aligned} \tag{1.3}$$

For $f(t) = 0$, $\overline{p} = \overline{p}_0 e^{-t/\tau_m}$. ($\tau_m$: momentum relaxation time, mean free time, transport scattering time.)

Remark Random scattering causes dissipation. It turns $p(t)$ to p_{ran} with the probability dt/τ_m, resulting the decay of $p(t)$. τ_m only counts effective collision which leads to momentum relaxation. Not all collision changes the e momentum in an efficient way.

Given the collision time τ_c, τ_m can be expressed as $\frac{1}{\tau_m} = \alpha_m \frac{1}{\tau_c}$, where α_m is the effectiveness of collision in destroying momentum. The mean free path can be expressed as $l = v_d \tau_m$, where v_d is the drift velocity. Low α_m: (1) smooth impurity (2) chiral state.

For a constant force, $\overline{p}(t) = \overline{p}_0 e^{-t/\tau_m} + \tau_m \overline{f}(1 - e^{-t/\tau_m})$. Consider an electromagnetic force, $\vec{\overline{f}} = -e(\vec{E} + \vec{v}_d \times \vec{B})$. By using $\vec{\overline{p}} = m\vec{v}_d$, one obtains

$$\dot{\vec{v}}_d = -\frac{e}{m}(\vec{E} + \vec{v}_d \times \vec{B}) - \frac{\vec{v}_d}{\tau_m} \tag{1.4}$$

For a steady (nonequilibrium) state, $\dot{\vec{v}}_d = 0$. After a time $t \gg \tau_m$, $m\vec{v}_d/\tau_m = -e(\vec{E} + \vec{v}_d \times \vec{B})$. For zero magnetic field, i.e. $\vec{B} = 0$, one obtains

$$\vec{v}_d = -\frac{e\tau_m}{m}\vec{E} = -\mu\vec{E} \tag{1.5}$$

where we define the mobility $\mu = e\tau_m/m$ characterizing the moving ability of e driven by $\vec{E}$. The relation between drift velocity $\vec{v}_d$ and $\vec{E}$ yields Ohm's law, $\vec{J} = \sigma_0\vec{E}$, $\sigma_0 = en_s\mu$, $\vec{J} = -e\vec{v}_d n_s = en_s\mu\vec{E}$, where n_s is the carrier density. Defining cyclotron frequency $\omega_c = eB/m$, we have $\mu B = eB\tau_m/m = \omega_c\tau_m$.

For a 2D sample with an electromagnetic field ($\vec{B}$ along the z-direction, $\vec{E}$ along the x-y plane),

$$\vec{E} = -\frac{m\vec{v}_d}{\tau_m e} + \vec{B} \times \vec{v}_d$$

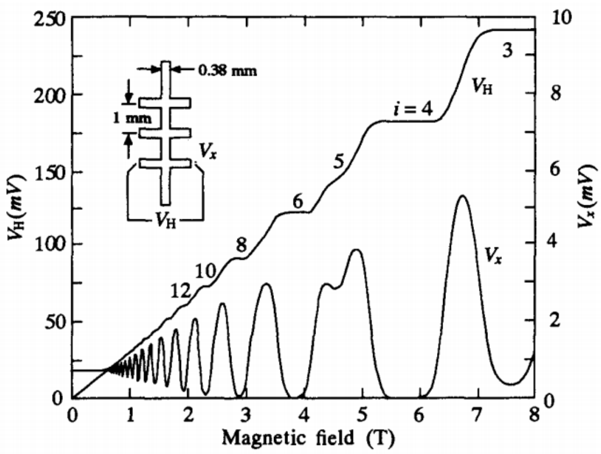
$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} -\frac{m}{\tau_m e} & -B \\ B & -\frac{m}{\tau_m e} \end{pmatrix} \begin{pmatrix} v_x \\ v_y \end{pmatrix} = \begin{pmatrix} -1/\mu & -B \\ B & -1/\mu \end{pmatrix} \begin{pmatrix} v_x \\ v_y \end{pmatrix} \tag{1.6}$$

$$\rightarrow \begin{pmatrix} E_x \\ E_y \end{pmatrix} = -\frac{1}{en_s} \begin{pmatrix} -1/\mu & -B \\ B & -1/\mu \end{pmatrix} \begin{pmatrix} J_x \\ J_y \end{pmatrix} = \sigma_0^{-1} \begin{pmatrix} 1 & \mu B \\ -\mu B & 1 \end{pmatrix} \begin{pmatrix} J_x \\ J_y \end{pmatrix}$$

The resistivity tensor reads

$$\rho = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{pmatrix} = \sigma_0^{-1} \begin{pmatrix} 1 & \mu B \\ -\mu B & 1 \end{pmatrix} \tag{1.7}$$

with the longitudinal resistivity $\rho_{xx} = \rho_{yy} = \sigma_0^{-1} = (en_s\mu)^{-1}$ and the Hall resistivity $\rho_{yx} = -\rho_{xy} = -\mu B/\sigma_0 = -B/(en_s)$.



The resistivity tensor describes the $\vec{E}$ field or voltage driven by a current. It benefits the measurement of

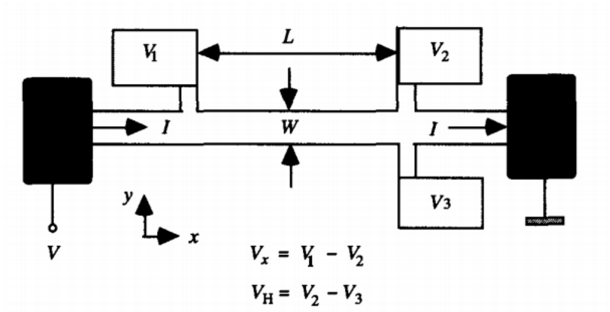
(1) carrier density, $\quad -en_s = dB/d\rho_{yx} \quad$ by Hall resistivity(HR)

(2) mobility, $\quad \mu = 1/(en_x\rho_{xx}) \quad$ by carrier density(CD)+longitudinal resistivity(LR)

It is also very convenient to measure the resistivity tensor. There are only two independent matrix elements in ρ. In experiments, we consider a rectangular sample. One can simply set $J_y = 0$, which gives $E_x = \rho_{xx}J_x$ and $E_y = \rho_{yx}J_x$, and then measure the longitudinal and Hall voltage drop by $V_x = E_xL$, $V_H = E_yW$, which gives $\rho_{xx} = \frac{V_x}{I}\frac{W}{L}$, $\rho_{yx} = \frac{V_H}{I}$ by using $I = J_xW$.

Remark ρ is favorable for experimental measurements, while σ is favorable for theoretical analysis.

For physical picture, it is more straightforward to imagine the response of electron movement or current to external fields. For theoretical analysis, there are different methods to directly calculate the current.



Rectangular Hall bar for magnetoresistance measurements.

Consider the conductivity tensor σ,

$$\begin{pmatrix} J_x \\ J_y \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \end{pmatrix} \quad \sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} \tag{1.8}$$

It is just the inverse of the resistivity tensor, $\sigma = \rho^{-1}$,

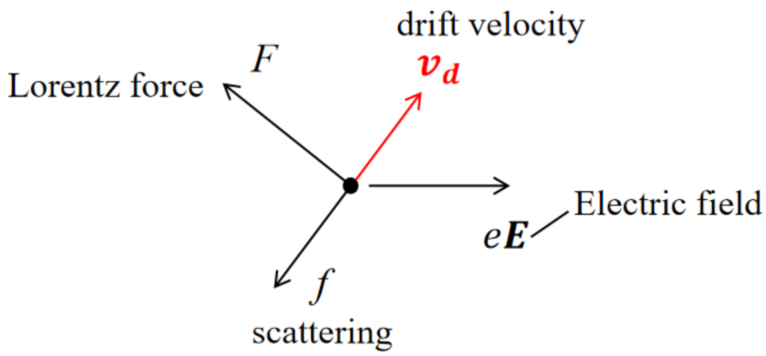
$$\begin{aligned} \sigma_{xx} = \sigma_{yy} &= \frac{\rho_{xx}}{\rho_{xx}^2 + \rho_{xy}^2} = \frac{\sigma_0}{1 + \mu^2 B^2} \\ \sigma_{xy} = -\sigma_{yx} &= -\frac{\rho_{xy}}{\rho_{xx}^2 + \rho_{xy}^2} = -\frac{\mu B \sigma_0}{1 + \mu^2 B^2} \end{aligned} \tag{1.9}$$

Remark In the presence of B, $\sigma_{xx} \neq \rho_{xx}^{-1}$. $\sigma_{xx} = \rho_{xx}^{-1}$ only for $B = 0$, in which σ and ρ are diagonal.

If we impose an $\vec{E}$ field along the x-direction, the current

$$\begin{aligned} J_x &= \sigma_{xx} E_x = \frac{\sigma_0}{1 + \mu^2 B^2} E_x \\ J_y &= \sigma_{yx} E_x = \frac{\sigma_0 \mu B}{1 + \mu^2 B^2} E_x \end{aligned} \tag{1.10}$$

Due to the $\vec{B}$ field, the current deviates from the direction of the $\vec{E}$ field by a **Hall angle** ϕ: $\tan\phi = \mu B = \omega_c \tau_m$.



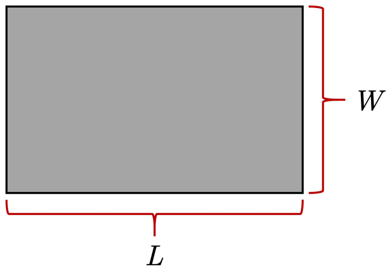
In the clean limit, $\tau_m, \mu \to \infty, J_x = 0, \sigma_{xx} = 0, \rho_{xx} = 0$. Thus only Hall current remains. The Hall conductivity $\sigma_{yx} = en_s/B, \rho_{yx} = -\sigma_{yx}^{-1}$. For $\mu \to \infty$, σ, ρ are anti-symmetric matrices. In general cases, μ is finite, both dissipation (finite τ_m) and B exist. Both σ and ρ take the general form, related to each other through inversion.

Remark Both σ_{xx}, ρ_{xx} are zero. $\sigma_{xx} = 0$, because no longitudinal current is driven; $\rho_{xx} = 0$, because no dissipation.

1.2 Why quantum and How?

For a homogeneous macroscopic sample, the conductivity σ is well defined through the conductance:

$$G = \sigma W/L. \tag{1.11}$$



This relation holds only in the ohmic regime. Physically, σ is an average effect of the random scattering of electrons, so that in the scale of the mean free path l, σ is no longer well defined.

The ohmic regime requires the dimensions of the conductor to be much larger than each of three characteristics length scales:

1. the de Broglie wave length λ_F, which is related to the kinetic energy of electrons
2. the mean free path l, which is related to the relaxation of the electron's momentum;
3. the phase relaxation length, l_φ, which is the distance for electron losing the phase coherence.

In mesoscopic systems, which typically range in size from nanometers (nm) to approximately 100 micrometers (μm), classical Drude model fails not only because $L \precsim l$, but also due to the enter of various quantum effect. In practice, mesoscopic transport can be conducted at extremely low temperatures, where quantum interference effect becomes dominant.

Quantum Effect involve:

- Identical particle: Fermi-Dirac distribution.
- Energy quantization: Transverse modes due to finite-size effect.
- Phase coherence: Interference effect.

Remark In quantum transport, some classical concepts remain true such as mean-free path. Also, in many cases, semiclassical picture can guide our pursuit for the solution with the quantum correlation.

Various quantum regimes are associated with characteristics lengths:

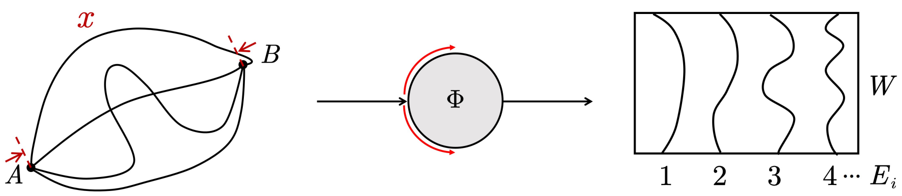
- sample size L;
- Fermi wave length λ_F;
- Mean free path l;
- Phase-coherence length λ_φ;
- Magnetic length $l_B = \sqrt{\hbar/eB}$;
- Localization length ξ.

Depending on the relation magnitudes of these lengths, the transport takes place in different scenarios:

- $L \ll l$, Ballistic regime;
- $L \gg l$, $l_\varphi \leq l$, Classical diffusion;
- $L \gg l$, $l_\varphi \gg l$, Quantum diffusion;
- $\lambda_F \sim L$, Finite size effect & level spacing;
- $L \gtrsim \xi$, Strong (Anderson) localization;
- $L \ll \xi$, weak localization;
- $l_B \gg l$, weak magnetic field limit;
- $l_B \ll l$, stronger magnetic field limit, Landau level dominant.

1.2.1 Physical Meanings of Typical Lengths

1. Mean free path l. No much difference from classical regime: $l = v_d \tau_m \to l = v_F \tau_m$. Electron near Fermi surface contribute $v_F = 3 \times 10^5 m/s$. Given $n_s = 5 \times 10^{11}/cm^2$ and $\tau_m = 100ps$, it follows that $l = 30\mu s$.
2. Fermi wave length $\lambda_F = 2\pi/k_F$. Its effect is revealed in two aspects:
   (a) Interference



   The expression for the phase factor is given by $e^{ik_F \cdot x}$. Consequently, when $x \geq \lambda_F$ and $l_\varphi \gg x$, dephasing occurs.
   The propagator can be expressed as $a \sim \sum_n e^{i\theta_n}$, with $\theta_n = \int_{C_n} k \cdot dx$. Consequently, there are two way to enhance interference: i) reduce the interference channels. ii) introduce phase-locking technique such that $\theta_n = \theta_{n'}$, such as TR symmetry, WL, WAL.

   (b) Level spacing if $W \sim \lambda_F$, finite size effect leads to level spacing.

$$\lambda_n = 2W/n \tag{1.12}$$

$$\Rightarrow \varepsilon_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\pi^2 \hbar^2}{2m} \frac{n^2}{W^2} \tag{1.13}$$

   Assuming that $W \sim 10\,\text{nm}$, it follows that $\Delta\varepsilon \sim 100\,\text{meV}$. Typical energy scale in mesoscopic transport is $1 \sim 10meV$. If $W \sim \lambda_F$, only the lowest one or two subbbands are relevant. Conversely, when $W \gg \lambda_F$, boundary condition is unimportant. One can use simply periodic boundary condition, and the transport shows 2D behavior.

3. Phase coherence (relaxation) length l_φ. Phase coherence is the most important parameter in quantum transport. Without phase coherence, most results can be obtained under Drude-Boltzmann taking into account Fermi-Dirac statistics.

Phase coherence time τ_φ:

$$\frac{1}{\tau_\varphi} = \frac{1}{\tau_c} \alpha_\varphi \tag{1.14}$$

where α_φ is the effectiveness of collision in destroying phase.

Question: *What is phase coherence? And how to destroying it?*

1.2.2 Phase Coherence

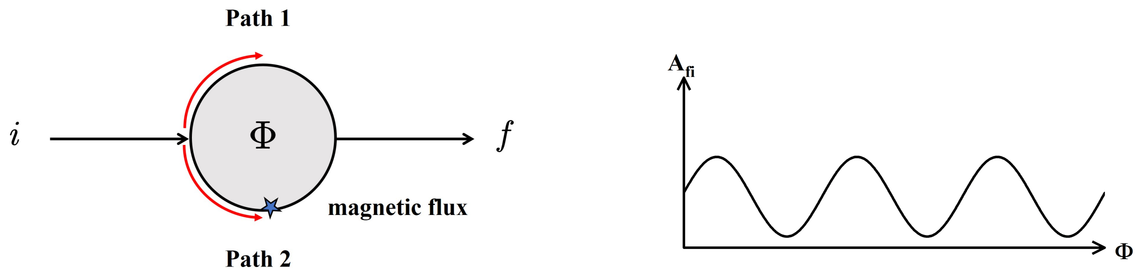
Quantum state superposition:

$$\psi = \sum_i \psi_i \tag{1.15}$$

$$\Rightarrow |\psi|^2 = \sum_i |\psi_i|^2 + \sum_{i \neq j} \psi_i^* \psi_j \tag{1.16}$$

where the interference effect arises from the second term in the final line.

Example 1.1



A simple case:

$$a_{fi} = a_1 + a_2 \tag{1.17}$$

$$\Rightarrow A_{fi} = |a_{fi}|^2 = |a_1|^2 + |a_2|^2 + a_1 a_2^* + a_1^* a_2 \tag{1.18}$$

where $a_1 = |a_1|e^{i\varphi_1}$ and $a_2 = |a_2|e^{i(\varphi_2+\varphi_B)}$[1], so that:

$$A_{fi} = |a_1|^2 + |a_2|^2 + |a_1 a_2| \left(e^{i\varphi_1 e^{-i\varphi_2 - i\varphi_B}} + c.c.\right) \tag{1.19}$$

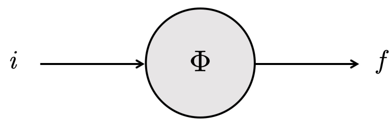
$$= |a_1|^2 + |a_2|^2 + 2|a_1 a_2| \cos(\varphi_1 - \varphi_2 - \varphi_B) \tag{1.20}$$

Thus, when $|a_1| = |a_2|$, the interference achieved is at its maximum.

Remark Quantum interference, Quantum measurement on ensemble. A single shot experiment cannot give interference: Two possible output : 0, or 1. 1 nA. 10^9 electrons transmit on surface in $1s$.

Ensemble average: Probability distribution $A_{fi}(\Phi)$. The distribution function contains interfering information, exhibiting oscillation with Φ. For a huge number of electrons, the relative fluctuation of average physical quantity is very small according to the law of large numbers.

Thus, the coherence status of the system can be determined using $A_{fi}(\Phi)$. (1) Coherence: For a fixed Φ, $A_{fi}(\Phi)$ does not fluctuate! (2) Decoherence: For a fixed Φ, $A_{fi}(\Phi)$ fluctuates!



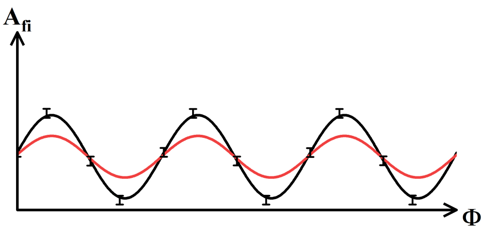


Figure 1.1: There are two-fold of average: 1. quantum average. 2. environment average.

$$A_{fi} = |a_1|^2 + |a_2|^2 + e^{-\tau/\tau_\varphi} 2|a_1 a_2| \cos(\varphi_1 - \varphi_2 - \varphi_B) \tag{1.21}$$

The factor $e^{-\tau/\tau_\varphi}$ lead to the reduction of coherent oscillation.

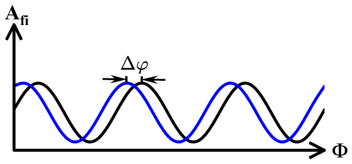
[1] The overall $U(1)$ phase is unimportant, which is also unknown for each electron.

Static impurity does not destroy phase coherence: Consider impurity along path 2. Then it will introduce additional phase $\Delta\varphi \sim Ut/\hbar$ by static scattering:

$$a_{fi} = a_1 + a_2 e^{i\varphi_B} e^{i\Delta\varphi} \tag{1.22}$$

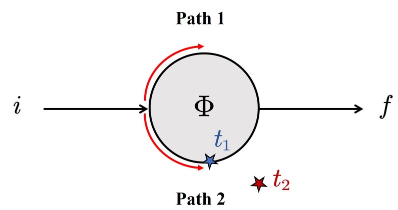
$$\Rightarrow A_{fi} = |a_1|^2 + |a_2|^2 + 2|a_1 a_2| \cos(\varphi_1 - \varphi_2 - \varphi_B - \Delta\varphi), \tag{1.23}$$

the oscillation phase shifts by $\Delta\varphi$, but its amplitude is unaffected



1.2.3 Decoherence

- **Decoherence scenario 1: classical randomness of environment**

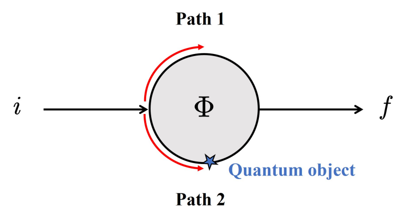


$$\langle A_{fi} \rangle = |a_1|^2 + |a_2|^2 + \langle |a_1 a_2| \left(e^{i\varphi_1} e^{-i\varphi_2 - i\varphi_B - i\Delta\varphi(t)} + c.c. \right) \rangle \tag{1.24}$$

$$= |a_1|^2 + |a_2|^2 + \langle 2|a_1 a_2| \cos\left(\varphi_1 - \varphi_2 - \varphi_B - \Delta\varphi(t)\right) \rangle \tag{1.25}$$

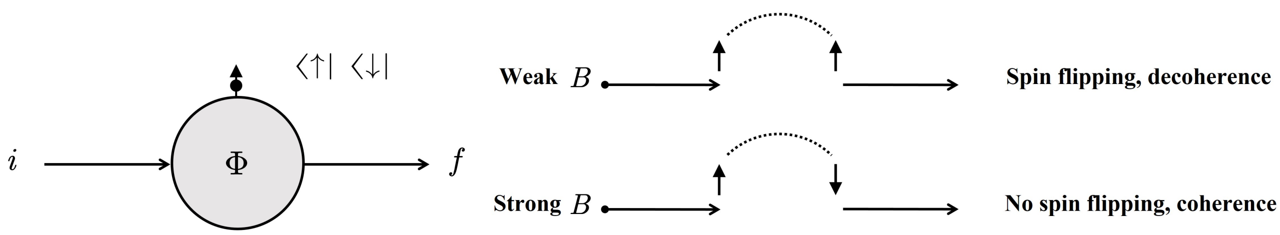
$$= |a_1|^2 + |a_2|^2 + 2|a_1 a_2| \int d\xi \, \cos\left(\varphi_1 - \varphi_2 - \varphi_B - \Delta\varphi(t)\right) f(\xi) \tag{1.26}$$

- **Decoherence scenario 2: intrinsic quantum fluctuation of environment**



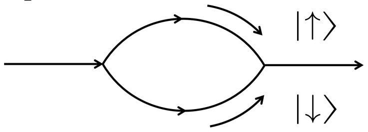
$$\text{Quantum object} \begin{cases} \text{electron-phonon interaction} \\ \text{electron-electron interaction} \\ \text{impurity with internal DOF} \end{cases}$$

Example 1.2 Here is an example for impurity with internal DOF. In the case of a weak magnetic field B, the



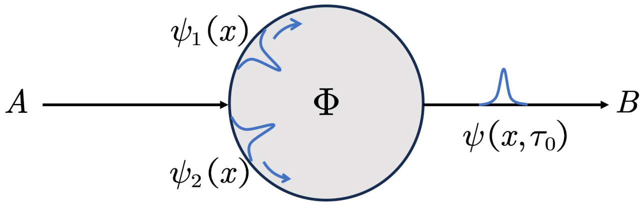
presence of a magnetic impurity induces spin flipping, leading to electron decoherence. Conversely, under a strong magnetic field B, spin flipping is absent, thus maintaining electron coherence.

Which-way experiment: As long as the which-way information can be obtained in principle by measuring the state of the scatterer, decoherence takes place.



Spin as a which-way detector

1.2.4 Equivalence between which-way picture & fluctuating scatterer



1.2.4.1 Which-way picture

Considering an initial state: $\tilde{\psi}(t=0) = [\psi_1(x)+\psi_2(x)]\otimes\chi_0(\eta)$. At time τ_0, the interference is examined, the wavefunction is an entangled state between electron and the environment[2]:

$$\tilde{\psi}(\tau_0) = \psi_1(x,\tau_0)\otimes\chi_1(\eta,\tau_0) + \psi_2(x,\tau_0)\otimes\chi_2(\eta,\tau_0). \tag{1.27}$$

The electron plus environment is a closed system, described by a pure, entangled state, $\tilde{\psi}(\tau_0)$. The measurement is performed on electron only, whose state is a mixed state by tracing out the DOF of the environment. For decoupled electron and environment:

$$|\psi|^2 = |\psi_1(x,\tau_0) + \psi_2(x,\tau_0)|^2 \tag{1.28}$$

$$= |\psi_1(x,\tau_0)|^2 + |\psi_2(x,\tau_0)|^2 + 2\mathrm{Re}[\psi_1^*\psi_2] \tag{1.29}$$

For entangled state:

$$|\psi|^2 = \mathrm{Tr}_\eta[\langle x|\,\tilde{\psi}\rangle\,\langle\tilde{\psi}|\,x\rangle] \tag{1.30}$$

$$= \mathrm{Tr}_\eta\left[(\psi_1(x,\tau_0)\otimes\chi_1(\eta,\tau_0) + \psi_2(x,\tau_0)\otimes\chi_2(\eta,\tau_0))\right.$$
$$\left.\times\,(\psi_1^*(x,\tau_0)\otimes\chi_1^*(\eta,\tau_0) + \psi_2^*(x,\tau_0)\otimes\chi_2^*(\eta,\tau_0))\right] \tag{1.31}$$

$$= \int d\eta\,(\psi_1\chi_1 + \psi_2\chi_2)(\psi_1^*\chi_1^* + \psi_2^*\chi_2^*) \tag{1.32}$$

$$= |\psi_1(x,\tau_0)|^2 \int d\eta\,\chi_1(\eta)\chi_1^*(\eta) + \psi_1(x,\tau_0)\psi_2^*(x,\tau_0)\int d\eta\,\chi_1(\eta)\chi_2^*(\eta)$$
$$+\,\psi_2(x,\tau_0)\psi_1^*(x,\tau_0)\int d\eta\,\chi_2(\eta)\chi_1^*(\eta) + |\psi_2(x,\tau_0)|^2\int d\eta\,\chi_2(\eta)\chi_2^*(\eta) \tag{1.33}$$

$$= |\psi_1(x,\tau_0)|^2 + |\psi_2(x,\tau_0)|^2 + 2\mathrm{Re}\left[\psi_1(x,\tau_0)\psi_2^*(x,\tau_0)\int d\eta\,\chi_1(\eta)\chi_2^*(\eta)\right] \tag{1.34}$$

The which-way information is encoded in $|\chi_1\rangle$, $|\chi_2\rangle$. The entangled state means that if electron chooses 1 path, then the detector is in state $|\chi_1\rangle$; is it chooses 2 path, then the detector is in state $|\chi_2\rangle$. $\langle\chi_1|\,\chi_2\rangle = 1$

[2]Here, the "environment" is a general concept, it can also be different DOF (such as spin) of the electron itself.

corresponds to a poor detector because which-way information cannot be reflected by $|\chi_1\rangle$, $|\chi_2\rangle$, one cannot tell which electron chooses $\langle\chi_1|\,\chi_2\rangle = 0$, then it is a perfect which-way detector, because the path of electron is completely reflected by $|\chi_1\rangle$, $|\chi_2\rangle$, which are orthogonal. Therefore, quantum interference, which is the result of an uncertainty in the path, is then lost.

Remark In this picture, the coherence time (phase-breaking time) τ_ϕ is the time in which the two interfering partial waves shift the environment into states orthogonal to each other, that is, when the environment has the information on the path the electron takes. [Y.Imry Mesoscopic physics].

1.2.4.2 The second picture

How the environment affects the partial waves rather than how the waves affect the environment (as a detector). Consider a static potential $(V(x))$, its effect on the electron wave is an accumulate phase

$$\Delta\phi = -\int V(x(t))dt/\hbar. \tag{1.35}$$

A static potential means it is a pure function of the DOF of electron, which gives a certain $\Delta\phi$. When V is not static, but created by the DOF of the environment, $\hat{V}$ becomes an operator. Thus its value is not longer well defined. The uncertainty of the value of $\hat{V}$ stems from the quantum uncertainty (fluctuation) in the state of the environment. Therefore, $\Delta\phi$ is also an operator, without definite value. $\Delta\phi$ now possesses a distribution function $P(\Delta\phi)$.

Consider the wave function:

$$\psi(\Delta\phi) = \psi_1 + e^{i\Delta\phi}\psi_2 \tag{1.36}$$

After average:

$$\langle\psi(\Delta\phi)\rangle = \psi_1 + \langle e^{i\Delta\phi}\rangle\psi_2 \tag{1.37}$$

$$\langle e^{i\Delta\phi}\rangle = \int p(\Delta\phi)e^{i\Delta\phi}d\Delta\phi \tag{1.38}$$

For probability:

$$\langle|\psi(\Delta\phi)|^2\rangle = |\psi_1|^2 + |\psi_2|^2 + \langle\big(e^{i\Delta\phi}\psi_1\psi_2^* + c.c.\big)\rangle \tag{1.39}$$

$$= |\psi_1|^2 + |\psi_2|^2 + \langle e^{i\Delta\phi}\rangle\psi_1^*\psi_2 + \langle e^{-i\Delta\phi}\rangle\psi_2^*\psi_1 \tag{1.40}$$

$$= |\langle\psi(\Delta\phi)\rangle|^2 \tag{1.41}$$

The decoherence arise from the summation of different $\Delta\phi$ terms, which are out of phase. $\langle e^{i\Delta\phi}\rangle$ tends to zero when $P(\Delta\phi)$ is slowly varying over a region much larger then 2π [3]. Then the interference is strongly suppressed.

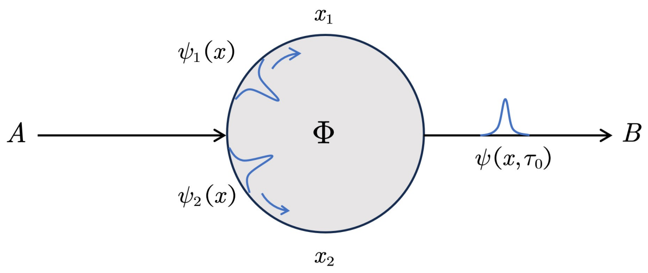
Remark In this picture, the phase breaking time is also the time in which the uncertainty in the phase becomes of the order of the interference periodicity.

1.2.4.3 equivalence between the two explanations

The equivalence between the two explanations is given by the equation: $\langle e^{i\Delta\phi}\rangle = \int d\eta\, \chi_1^*(\eta)\chi_2(\eta)$. It is rather a beautiful relation. When the environment measures the path taken by the electron, with $\langle\bar{\chi_1}\chi_2\rangle = 0$, it induces a phase shift whose uncertainty is of the order of 2π. The statement holds only when the environment is itself quantum, rather than some intended tuning of a classical parameter to be random.

[3] In the Feynman-Vernon terminology, $\langle e^{i\Delta\phi}\rangle$ is the influence functional.

Consider the Hamiltonian of the environment $H_{env}(\eta, p_\eta)$, and that for the interaction $V(\chi_{1,2}(t), \eta)$, H_0 for electron satisfies $[H_0, V] = 0$.



Start with the state:

$$\tilde{\psi}(t=0) = [\psi_1(x) + \psi_2(x)] \otimes \chi_0(\eta) \tag{1.42}$$

We have:

$$\tilde{\psi}(\tau_0) = \psi_1(x,\tau_0)\hat{T}\exp\left[\frac{1}{i\hbar}\int_0^{\tau_0} dt\,(H_{env}+V)\right]\chi_0(\eta) + \psi_2(x,\tau_0)\hat{T}\exp\left[\frac{1}{i\hbar}\int_0^{\tau_0} dt\,(H_{env}+V)\right]\chi_0(\eta) \tag{1.43}$$

Interaction picture:

$$V_I(t) \equiv e^{iH_{env}t}V(x_{1,2}(t),\eta)e^{-iH_{env}t} \tag{1.44}$$

Consider only the path 2 where interaction take place.

$$\tilde{\psi}(\tau_0) = \psi_1(x,\tau_0) \otimes e^{-iH_{env}\tau/\hbar}\chi_0(\eta) + \psi_2(x,\tau_0) \otimes e^{-iH_{env}\tau/\hbar}\hat{T}\exp\left[-i\int_0^{\tau_0}\frac{dt}{\hbar}V_I(x_2(t),\eta)\right]\chi_0(\eta) \tag{1.45}$$

Then the interference term is:

$$\langle\chi_0|\,\hat{T}\exp\left[-i\int_0^{\tau_0}\frac{dt}{\hbar}V_I(x_2(t),\eta)\right]|\chi_0\rangle = \langle\chi_1|\,\chi_2\rangle = \langle\chi_0|\,\chi_2\rangle = \int \chi_1^*(\eta)\chi_2(\eta)d\eta \tag{1.46}$$

It means the interference of electron is affected by the state evolution of the environment. The latter is due to the interaction with the electron. Specifically, when $\langle\chi_1|\,\chi_2\rangle = 0$, the which-way information is fully known by the environment, which destroys the interference.

The interpretation in terms of phase uncertainty is also obvious. The unitary operator $\hat{T}\exp\left[-i\int_0^{\tau_0}\frac{dt}{\hbar}V_I(x_2(t),\eta)\right] = e^{i\Delta\hat{\phi}}$ can be understood as a quantum operator for phase shift $\Delta\hat{\phi}$. Since the environment is a quantum object, its action on the electron exhibits quantum fluctuation. In many cases, $P(\delta\phi)$ is a normal distribution, then

$$\langle e^{i\Delta\phi}\rangle = e^{i\langle\Delta\phi\rangle - \frac{1}{2}\langle\delta\phi^2\rangle} \tag{1.47}$$

where the term $\langle\Delta\phi\rangle$ represents the average phase, while the term $\langle\delta\phi^2\rangle$ induces decoherence.

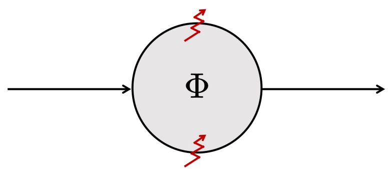
Question: *Fluctuating scatterer must lead to decoherence?*

Answer: *No! The fluctuation should be uncorrelated.*

Taking into account that the fluctuations in paths 1 and 2 are identical:

$$\hat{a}_{fi} = a_1 e^{i\Delta\varphi} + a_2 e^{i\varphi_B}e^{i\Delta\varphi} \tag{1.48}$$

$$= e^{i\Delta\varphi}(a_1 + a_2 e^{i\varphi_B}) \tag{1.49}$$



Although $\Delta\varphi$ is random, it is just an overall phase, unimportant

$$A_{fi} = |\hat{a}_{fi}|^2 = \langle e^{i(\Delta\varphi - \Delta\varphi)}\rangle\,(|a_1|^2 + |a_2|^2 + \cdots) = (|a_1|^2 + |a_2|^2 + \cdots) \tag{1.50}$$

Physical scenario: long wavelength phonon, energy $\hbar\omega$. The coherence time τ_ϕ, during which electron undergoes τ_{ϕ/τ_c} collision. The energy uncertainty is (like diffusion in ε-space)

$$(\Delta\varepsilon)^2 = (\hbar\omega)^2(\tau_\phi/\tau_c), \tag{1.51}$$

the phase factor is $e^{\frac{\varepsilon t}{i\hbar}}$, so the phase uncertainty

$$\Delta\varphi = \Delta\varepsilon\tau_\phi/\hbar \sim 1 \tag{1.52}$$

$$\Rightarrow \hbar\omega(\tau_\phi/\tau_c)^{\frac{1}{2}} = \bar{h}/\tau_\phi \tag{1.53}$$

$$\Rightarrow \omega^2\tau_\phi/\tau_c = \tau_\phi^{-2} \Rightarrow \tau_\phi \sim (\tau_c/\omega^2)^{\frac{1}{3}} \tag{1.54}$$

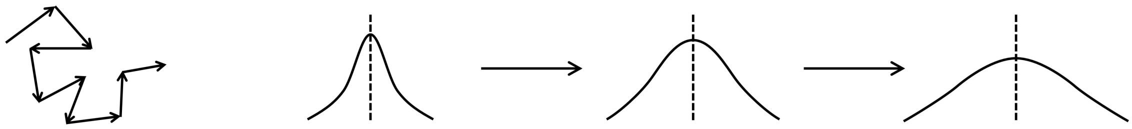
As $\omega\tau_c < 1$, than $\tau_\phi > \tau_c$. Low frequency phonons are less effective in relaxing phase.

1.2.5 Phase-coherence length l_φ

In low-mobility conductors the phase-coherence time is measured by weak localization experiments.

Question: *How τ_φ relates to l_φ?*

Answer: *we need to address this question by considering two distinct cases:*



elastic scattering **Diffusion**

(i) High-mobility semiconductors: $\tau_\varphi \sim \tau_m$, ballistic within τ_φ, $L_\varphi = v_F\tau_\varphi$.

(ii) Low-mobility samples: $\tau_\varphi \gg \tau_m$, diffusive within τ_φ.
Random walk: average displacement is zero. $N = \frac{\tau_\varphi}{\tau_m}$ steps. $|x_j| = v_F\tau_m\cos(\theta)$ for each step. $\langle x_N\rangle = \sum_{j=1}^{N}\langle x_j\rangle = 0$.
$\langle x_N\rangle = 0$ but $\langle x_N^2\rangle \neq 0$.

$$\langle x_N^2\rangle = \langle\left(\sum_{j=1}^{N} x_J\right)^2\rangle = \langle\sum_{j=1}^{N} x_j^2\rangle + \langle\sum_{i\neq j} x_i x_j\rangle \tag{1.55}$$

$$= \sum_{j=1}^{N}\langle x_j^2\rangle + \sum_{i\neq j}\langle x_i\rangle\langle x_j\rangle \tag{1.56}$$

$$= N\langle x_j^2\rangle \tag{1.57}$$

$$= N(v_F\tau_m)^2\langle\cos^2(\theta)\rangle \tag{1.58}$$

$$\Rightarrow \langle x_N^2\rangle = l_\varphi^2 = \frac{\tau_\varphi}{\tau_m}(v_F\tau_m)^2\langle\cos^2\theta\rangle \tag{1.59}$$

$$= \tau_m(v_F\tau_m)^2\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\cos^2\theta = v_F^2\tau_m\tau_\varphi/2 \tag{1.60}$$

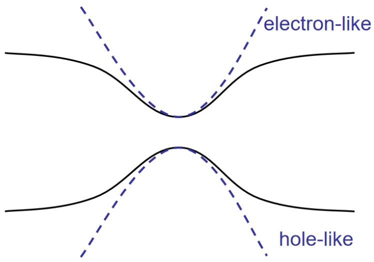
$$= D\tau_\varphi \tag{1.61}$$

where $D = v_F^2\tau_m/2$ is the diffusion coefficient.

1.3 Effective model

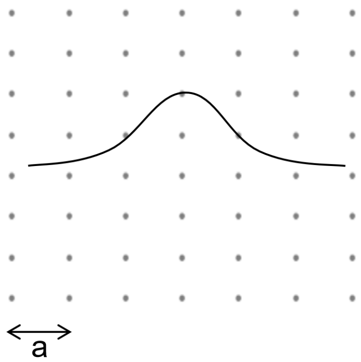
1.3.1 $k \cdot p$ model

The charge carriers in a metal/semiconductor are not (bare) electrons, but quasi-particles. (effect due to periodic lattice potential, interaction, etc.)



Effective mass description for semiconductor.

We only care about the length scale $l \gg a$, where a is the lattice constant, corresponding to the energy scale much smaller than the band width.



By choosing a $\vec{k}_0$, we can write the wave function as $\Psi = e^{i\vec{k}_0 \cdot \vec{r}} e^{i\vec{k}(\varepsilon) \cdot \vec{r}}$, which gives

$$H\Psi = E\Psi = [E_0(k_0) + \varepsilon(\vec{k})]\Psi \rightarrow H_{eff}(\vec{k}) e^{i\vec{k}\cdot\vec{r}} = \varepsilon(\vec{k}) e^{i\vec{k}\cdot\vec{r}} \tag{1.62}$$

For semiconductor, we use effective mass m^*, $[E_c + \frac{(i\hbar\nabla + e\vec{A})^2}{2m^*} + U(\vec{r})]\psi(\vec{r}) = \varepsilon\psi(\vec{r})$, where E_c is the reference energy of band edge, $\vec{A}$ is the vector potential, and U is the electric potential.

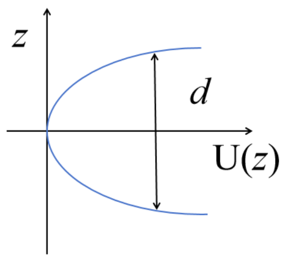
Remark Remark: The effective mass works only when $\vec{A}(\vec{r})$ and $\vec{U}(\vec{r})$ vary very smoothly in the scale of a. Otherwise, this description fails. Mathematically, the $k \cdot p$ perturbation method can be applied to any k point. However, the expanding point is chosen to be high-symmetry point such that the effective Hamiltonian possesses a simple form. Otherwise, the $k \cdot p$ method can hardly simplify the problem.

For Dirac Fermions (Graphene, Weyl semital), $H_{Dirac} = v_0 \vec{\sigma} \cdot (\vec{p} + e\vec{A})$.

1.3.2 subbands:finite-size effect

Consider a confinement in z-direction on a scale d. The wave function reads

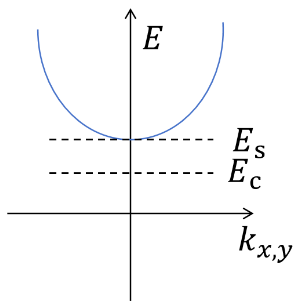
$$\Psi(\vec{r}) = \phi_n(z) e^{ik_x x} e^{ik_y y} \Longrightarrow E = E_c + \varepsilon_n + \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2) \tag{1.63}$$



where ε_n is the discrete energy in z-direction, $\Delta\varepsilon_n \sim \Delta k_z^2 \sim (\pi/d)^2$. For a thin film $d \to 0$, only $n = 1$ is relevant, which gives $[E_s + \frac{(i\hbar\nabla + e\vec{A})^2}{2m^*} + U(\vec{r})]\psi(\vec{r}) = \varepsilon\psi(\vec{r})$, where $E_s = E_c + \varepsilon_1$.

1.3.3 band diagrams

For free electron gas, $U = 0$, $\vec{A} = 0$, $\Psi(x, y) = e^{ik_x x} e^{ik_y y}$, $E = E_s + \frac{\hbar^2}{2m}(k_x^2 + k_y^2)$.



1.3.4 DOS (density of states)

The total number of states is

$$N_T(E) = 2 \times \frac{S}{4\pi^2} \int_{E_s}^{E} 2\pi k dk = \frac{mS}{\pi\hbar^2}(E - E_s) \tag{1.64}$$

The DOS is

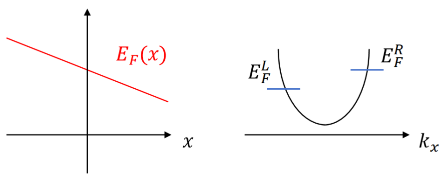
$$N(E) = \frac{1}{S}\frac{dN_T(E)}{dE} = \frac{m}{\pi\hbar^2}\theta(E - E_s) \tag{1.65}$$

Typical value for GaAs: $m^* = 0.07m_e$, $N(E) = 2.9 \times 10^{10} / \, cm^2 \cdot$ meV.

1.3.5 degenerated v.s. non-degenerated conductors

Fermi distribution: $f_0(E) = \frac{1}{1+e^{(E-E_F)/kT}}$ for equilibrium states.

Remark Remark: Away from equilibrium, the system has no common Fermi energy. Instead, we may have local quasi-Fermi level, which can vary spatially and can be different for different groups of states even at the same spatial location.



Two limits: (1) high temperature, non-degenerate limit, $e^{(E_s-E_F)/kT} \gg 1 \Rightarrow f_0(E) \simeq e^{-(E-E_F)/kT}$. (2) low temperature, degenerate limit, $e^{(E_s-E_F)/kT} \ll 1 \Rightarrow f_0(E) \simeq \theta(E-E_F)$. Relate the equilibrium electron density n_s to E_F,

$$n_s = \int N(E) f_0(E) dE = \frac{m}{\pi\hbar^2}(E_F - E_s) = N_s(E_F - E_s) \tag{1.66}$$

At low temperatures the conductance is determined entirely by electrons with energy close to E_F. Define the Fermi wavenumber k_F,

$$E_F - E_s = \frac{\hbar^2 k_F^2}{2m} \Rightarrow k_F = \frac{1}{\hbar}\sqrt{2m(E_F - E_s)} = \sqrt{2\pi n_s} \tag{1.67}$$

The Fermi velocity is $v_F = \hbar k_F / m$.

✍ **Exercise 1.1** Calculate the DOS for 2D & 3D Dirac fermion using the Hamiltonians below:

$$H_{2D} = \hbar v(\sigma_x k_x + \sigma_y k_y)$$
$$H_{3D} = \hbar v(\sigma_x k_x + \sigma_y k_y + \sigma_z k_z)$$

Solution *Hamiltonian:*

$$\begin{aligned} H_{2D} &= \hbar v \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} k_x + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} k_y \right] \\ &= \hbar v \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} \\ H_{3D} &= \hbar v \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} k_x + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} k_y + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} k_z \right] \\ &= \hbar v \begin{pmatrix} k_z & k_x - ik_y \\ k_x + ik_y & -k_z \end{pmatrix} \end{aligned}$$

Eigenvalue equation:

$$\begin{aligned} \det \begin{pmatrix} -E_{2D} & \hbar v(k_x - ik_y) \\ \hbar v(k_x + ik_y) & -E_{2D} \end{pmatrix} &= 0 \\ \Rightarrow E_{2D} = \pm\hbar v\sqrt{k_x^2 + k_y^2} &= \pm\hbar v|k| \\ \det \begin{pmatrix} \hbar v k_z - E_{3D} & \hbar v(k_x - ik_y) \\ \hbar v(k_x + ik_y) & -\hbar v k_z - E_{3D} \end{pmatrix} &= 0 \\ \Rightarrow E_{3D} = \pm\hbar v\sqrt{k_x^2 + k_y^2 + k_z^2} &= \pm\hbar v|k| \end{aligned}$$

Let $N_{2D/3D}$ represent the number of states, then the density of states (DOS) can then be determined as *follows:*

$$\begin{aligned} dN_{2D} &= 2\frac{S}{(2\pi)^2}2\pi|k|d|k| \\ &= 2\frac{S}{(2\pi)^2}2\pi E dE/(\hbar v)^2 \\ \Rightarrow g_{2D}(E) &= \frac{1}{S}\frac{dN_{2D}(E)}{dE} = \frac{E}{\pi(\hbar v)^2} \\ dN_{3D} &= 2\frac{V}{(2\pi)^3}4\pi|E|^2 d|E|/(\hbar v)^3 \\ \Rightarrow g_{3D}(E) &= \frac{1}{V}\frac{dN_{3D}(E)}{dE} = \frac{E^2}{(\pi)^2(\hbar v)^3} \end{aligned}$$

1.4 High-filled magnetoresistance (Longitudinal)

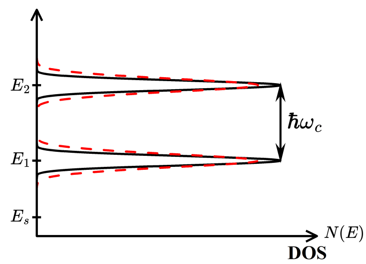
From Drude model, we see that for a single band model, there is no magnetoresistance. However, as B increases, oscillations show up in the longitudinal resistance ρ_{xx}, which is referred to as Shubnikov-de Hass (SdH) oscillations. Drastic modification of DOS due to forming Landau levels.

In the absence of B, the expression for $N_s(E)$ is given by $N_s(E) = \frac{m}{\pi\hbar^2}\theta(E - E_s)$. Conversely, when B is present, $N_s(E)$ is given by:

$$N_s(E) = \hbar\omega_c \frac{m}{\pi\hbar^2}\sum_{n=0}^{\infty}\delta\left[E - E_s - (n+\frac{1}{2})\hbar\omega_c\right] \tag{1.68}$$

$$= \frac{\hbar e B}{m}\frac{m}{\pi\hbar^2}\sum_{n=0}^{\infty}\delta\left[E - E_s - (n+\frac{1}{2})\hbar\omega_c\right] \tag{1.69}$$

$$= \frac{2eB}{h}\sum_{n=0}^{\infty}\delta\left[E - E_s - (n+\frac{1}{2})\hbar\omega_c\right] \tag{1.70}$$



Original quantum states within $\hbar\omega_c$ are swallowed into one degenerate Landau level.

For a given electron density n_s, we can calculate the number of occupied Landau level as:

$$N_{occ} = n_s/(2eB/h). \tag{1.71}$$

For $B = 2T$, it follows that $2eB/h = 9.6 \times 10^{10}\ /cm^2$. Additionally, when $n_s = 5 \times 10^{11}\ /cm^2$, we obtain $n_s/(2eB/h) = 5.2$.

Five Landau levels are fully occupied, sixth one is partially occupied. The resistivity ρ_{xx} goes through a max every time this number is a half-integer and the Fermi-energy lies at the center of a Landau level.

For two successive peaks with B_i, B_{i+1} (each with a half-filled LL):

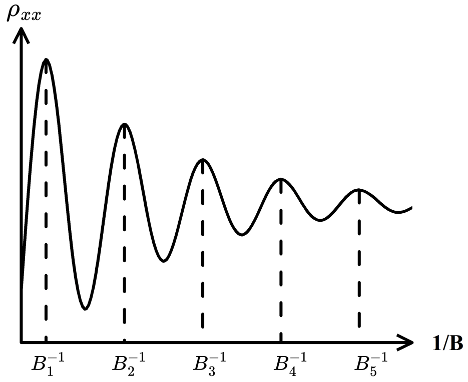
$$\frac{n_s}{2eB_i/h} - \frac{n_s}{2eB_{i+1}/h} = 1 \tag{1.72}$$

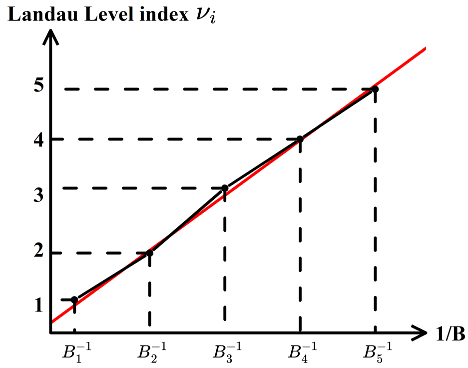
$$\Rightarrow n_s = \frac{2e}{h}\frac{1}{B_i^{-1} - B_{i+1}^{-1}} \tag{1.73}$$

$$\Rightarrow B_i^{-1} - B_{i+1}^{-1} = \frac{2e}{hn_s} \tag{1.74}$$

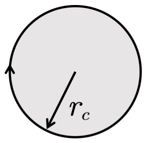
We define $\nu_i = \frac{n_s h}{2e}B_i$.

1.4.1 Landau Levels Onsager-Lifshitz Quantization





Semiclassic picture: $r_c = v/\omega_c$. Quantization version:



cyclotron motion

$$2\pi r_c mv = 2\pi r_c p = nh \tag{1.75}$$

$$\Rightarrow mv^2 = n\hbar\omega_c \tag{1.76}$$

and discrete energies $E_n - E_s = n\hbar\omega_c$, qualitatively correct except for a shift due to quantum fluctuation

$$E_n - E_s = (n + \frac{1}{2})\hbar\omega_c \tag{1.77}$$

What is the Onsager-Lifshitz quantization?

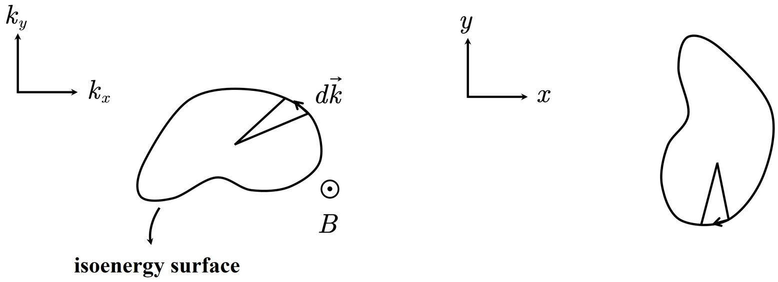
(1) Generalized Bohr-Sommerfeld QC in a magnetic field.

(2) Landau levels for quasi-particle with general dispersion.

$$\begin{cases} \hbar\frac{d\vec{k}}{dt} = -e\vec{v}\times\vec{B} \\ \vec{v}(\vec{k}) = \frac{1}{\hbar}\nabla_k\varepsilon(\vec{k}) \end{cases} \tag{1.78}$$

$$\Rightarrow \hbar(\vec{k} - \vec{k}_0) = -e(\vec{r} - \vec{r}_0)\times\vec{B} \tag{1.79}$$

$$\Rightarrow |\vec{r}' - \vec{r}_0| = \eta|\vec{k} - \vec{k}_0| \tag{1.80}$$



2D case

Onsager-Lifshitz quantization:

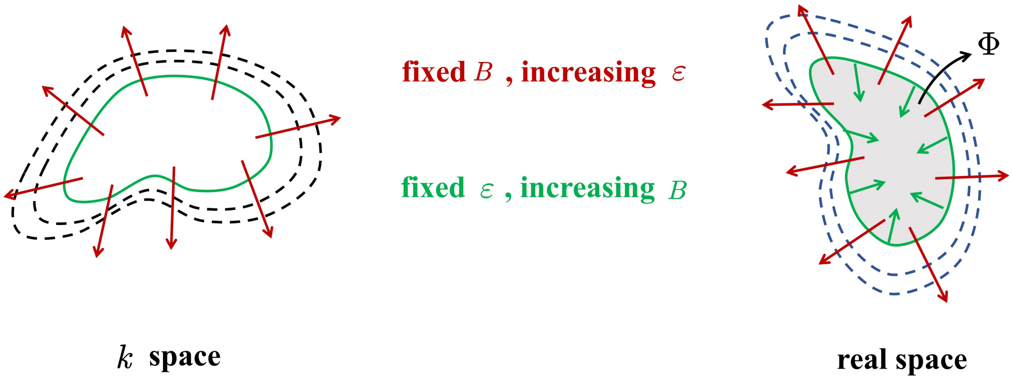
$$\oint \vec{p}\cdot d\vec{q} = (n+\gamma)\hbar \qquad \begin{cases} \gamma = \frac{1}{2} & \text{no Berry phase} \\ \gamma = 0 & \pi \text{ Berry phase} \end{cases} \tag{1.81}$$

Here, $\vec{p} = \hbar\vec{k} - e\vec{A}$, ($\hbar\vec{k} = \vec{p} + e\vec{A}$ appears in H) represents the canonical momentum, while $\vec{q} = \vec{r}$ denotes the canonical coordinate.

$$\oint(\hbar\vec{k}+e\vec{A})\cdot\vec{r}=\oint(\hbar\vec{k}_0-e(\vec{r}-\vec{r}_0)\times\vec{B})\cdot d\vec{r}-\oint e\vec{A}\cdot d\vec{r} \tag{1.82}$$
$$=-e\oint(\vec{r}\times\vec{B})\cdot d\vec{r}-e\oint\vec{A}\cdot d\vec{r} \tag{1.83}$$
$$=-e\oint\vec{B}\cdot(d\vec{r}\times\vec{r})-e\oiint(\nabla\times\vec{A})\cdot d\vec{S} \tag{1.84}$$
$$=e\oiint\vec{B}\cdot(\vec{r}\times d\vec{r})-e\oiint\vec{B}\cdot d\vec{S} \tag{1.85}$$
$$=2e\oiint\vec{B}\cdot d\vec{S}-e\oiint\vec{B}\cdot d\vec{S}=e\oiint\vec{B}\cdot d\vec{S}=e\Phi \tag{1.86}$$
$$\Rightarrow\Phi=(n+\gamma)\frac{h}{e}\qquad S_n=(n+\gamma)\frac{h}{eB} \tag{1.87}$$

Dual (momentum) space:

$$S_k^n=\eta^{-2}S_n=\frac{e^2B^2}{\hbar^2}(n+\gamma)\frac{h}{eB}=(n+\gamma)\frac{2\pi eB}{\hbar} \tag{1.88}$$



Example 1.3 Normal electron:

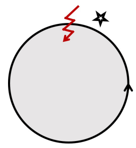
$$\begin{cases}\varepsilon=\frac{\hbar^2}{2m}(k_x^2+k_y^2), & r=\frac{1}{2}\\ S_k=\pi k^2=(n+\frac{1}{2})\frac{2\pi eB}{\hbar}, & n=0,1,2\ldots\end{cases} \tag{1.89}$$
$$\Rightarrow\varepsilon_n=\frac{\hbar^2}{2m}(n+\frac{1}{2})\frac{2eB}{\hbar}=(n+\frac{1}{2})\hbar\omega_c,\qquad\omega_c=\frac{eB}{m} \tag{1.90}$$

Example 1.4 Dirac fermion:

$$\begin{cases}\varepsilon^D=\pm\hbar vk=\pm\hbar v\sqrt{k_x^2+k_y^2}, & r=0\\ S_k=\pi k^2=n\frac{2\pi eB}{\hbar}\end{cases} \tag{1.91}$$
$$\Rightarrow k=\sqrt{\frac{2eB}{\hbar}|n|} \tag{1.92}$$
$$\Rightarrow\varepsilon_n^D=\pm\hbar v\sqrt{\frac{2eB}{\hbar}|n|}=\mathrm{sgn}(n)\sqrt{2e\hbar v^2|n|B},\qquad n=0,\pm1,\pm2\ldots \tag{1.93}$$

1.4.2 Physical condition for the Landau level regime[4]?

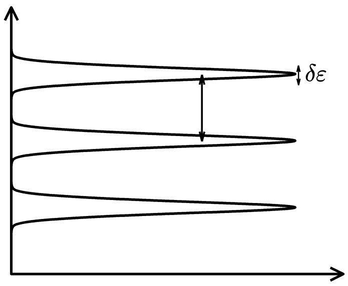
[4] Here the regime is the high-field regime (quantum regime)



In the ideal case, Landau levels will form for arbitrarily small B. In reality, an electron should be able to complete at least a few cyclotron orbits before losing its momentum due to scattering.

$$\omega_c^{-1} \ll \tau_m \Rightarrow \hbar\omega_c \gg \hbar/\tau_m \tag{1.94}$$

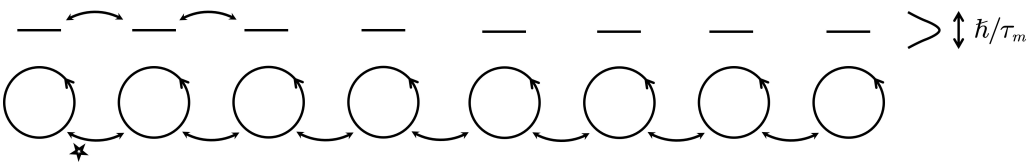
One can deduce the broadening of Landau levels. To see the levels, their broadening should be small than level spacing. By applying $\omega_c = eB/m$ and $\mu = e\tau_m/m$, the requirement becomes $B \gg \mu^{-1}$.



Conclusion *SdH oscillations are visible at longer magnetic fields for high mobility samples.*

Remark Graphene has very high mobility, quantum Hall effect can be observed even at room temperatures.

1.4.3 Flat-band (Landau levels) cannot conduct



1.4.4 Low field MR and high field MR both measure n_s

Usually $n_s^{\text{SdH}} < n_s^{\text{Low-field}}$, wherein n_s^{SdH} is influenced by mobility, while $n_s^{\text{Low-field}}$ remains unaffected by scattering.

1.5 Transverse modes (magneto-electric subbands)

In mesoscopic conductors, one or more directions are narrow. Electrons cannot move in those directions, and energies are discretized into separated energy levels. These modes all called transverse modes, analogous to the transverse modes of EM waves.

Consider a rectangular conductor, uniform in the x-direction, with confining potential $U(y)$:

$$[E_s + \frac{(i\hbar\nabla + e\vec{A})^2}{2m} + U(\vec{r})]\psi(\vec{r}) = E\psi(\vec{r}) \tag{1.95}$$

Consider a uniform B field in z direction. We choose the Landau gauge, $\vec{A} = (-By, 0, 0)$ (translation symmetry in x direction). Thus

$$[E_s + \frac{(p_x^2 + eBy)^2}{2m} + \frac{p_y^2}{2m} + U(\vec{r})]\psi(\vec{r}) = E\psi(\vec{r}) \tag{1.96}$$

where $p_x = -i\hbar\frac{\partial}{\partial x}$, $p_y = -i\hbar\frac{\partial}{\partial y}$. Ansatz:

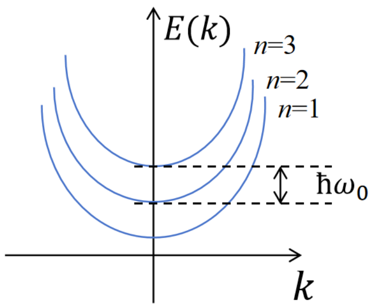
$$\psi(x,y) = \frac{1}{L}e^{ikx}\chi(y), \quad [E_s + \frac{(\hbar k + eBy)^2}{2m} + \frac{p_y^2}{2m} + U(\vec{r})]\chi(y) = E\chi(y) \tag{1.97}$$

For parabolic potential $U(y) = \frac{1}{2}mw_0^2y^2$ yields analytic solution, which is qualitatively correct.

1.5.1 $U \neq 0, B = 0$ (capture the main features of open boundary condition)

$$\begin{aligned} &[E_s + \frac{(\hbar k)^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega_0^2y^2]\chi(y) = E\chi(y) \\ &E(n,k) = E_s + \frac{\hbar^2k^2}{2m} + (n+\frac{1}{2})\hbar\omega_0, n = 0,1,2... \end{aligned} \tag{1.98}$$

$\chi_{n,k}(y) = u_n(q), q = \sqrt{m\omega_0/\hbar}y$, $u_n(q) = e^{-q^2/2}H_n(q)$, where $H_n(q)$ is the Hermit polynomial. $H_0(q) = \frac{1}{\pi^{1/4}}, H_1(q) = \frac{\sqrt{2}q}{\pi^{1/4}}, H_2(q) = \frac{2q^2-1}{\sqrt{2}\pi^{1/4}}$. The velocity for the nth mode: $v(n,k) = \frac{1}{\hbar}\frac{\partial E(n,k)}{\partial k} = \frac{\hbar k}{m}$.



For tight confinement in z-direction (5-10nm), $\Rightarrow \hbar\omega_0 \sim 100$meV. Only one or two bands are occupied. Confinement in y-direction is relatively weak, so subband spacing is much smaller and there may be many subbands occupied. There subbands are referred to as transverse modes.

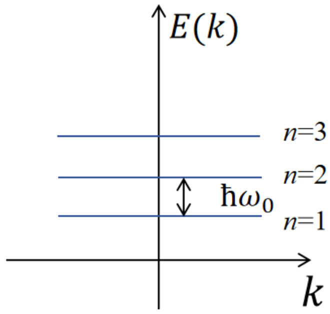
Remark Remark: If the confinement is so weak and the level spacing is much smaller than the interested energy scale such as E_F, then the open boundary condition is unimportant to the physics, one can then use the periodic condition and k_y can be regarded as a good quantum number.

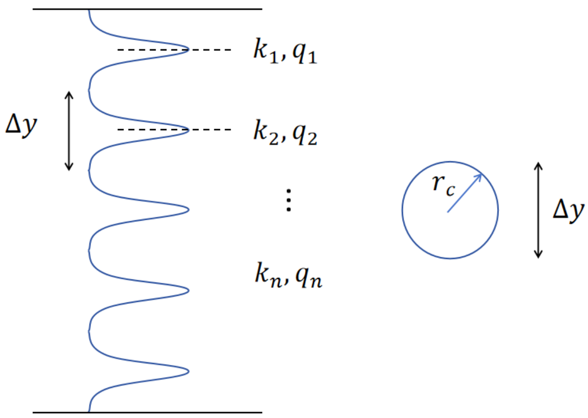
1.5.2 $U = 0, B \neq 0$: Landau level problem

$$\begin{aligned} &[E_s + \frac{(\hbar k + eBy)^2}{2m} + \frac{p_y^2}{2m}]\chi(y) = E\chi(y) \\ &[E_s + \frac{p_y^2}{2m} + \frac{1}{2}m\omega_c^2(y+y_k)^2]\chi(y) = E\chi(y) \end{aligned} \tag{1.99}$$

where $\omega_c = \frac{eB}{m}, y_k = \frac{\hbar k}{eB}$. $\chi_{n,k}(y) = u_n(q+q_y), E(n,k) = E_s + (n+\frac{1}{2}\hbar\omega_c), q = \sqrt{m\omega_c/\hbar}y, q_k = \sqrt{m\omega_c/\hbar}y_k$. ($\omega_0 \to \omega_c$ compared to the previous case).

$v(n,k) = \frac{1}{\hbar}\frac{\partial E(n,k)}{\partial k} = 0$. The wave packet cannot move because of zero dispersion. Consider $\psi_0(x,y) = \int \frac{dk}{2\pi}f(k)e^{ikx}\chi_{n,k}(y)$ (constructed with the nth Landau level), $\psi(x,y,t) = e^{\frac{Ht}{i\hbar}}\psi_0(x,y) = \psi_0(x,y)e^{-in\omega_ct}$, and the overall phase $e^{-in\omega_ct}$ is unimportant. $u_n(q+q_k) = e^{-(q+q_k)^2/2}H_n(q+q_k)$. The spatial extent of each wavefunction in the y-direction is approximated as $\Delta q^2 \sim 1$, $m\omega_c/\hbar\Delta y^2 \sim 1 \Rightarrow \Delta y \sim \sqrt{\frac{\hbar}{m\omega_c}} = \frac{\sqrt{\hbar\omega_c/m}}{\omega_c} \sim \frac{v}{\omega_c} = r_c \Rightarrow \frac{1}{2}mv^2 = \frac{1}{2}\hbar\omega_c$.





Degeneracy of Landau levels: (1) $N = \frac{mS}{\pi\hbar^2} \times \hbar\omega_c = \frac{eBS}{\pi\hbar}$. (2) $\Delta k = \frac{2\pi}{L}, \Delta y_k = \frac{\hbar\Delta k}{eB} = \frac{2\pi\hbar}{eBL}, N = \frac{W}{\Delta y_k} \times 2(spin) = \frac{2W}{2\pi\hbar}eBL = \frac{eBS}{\pi\hbar}$ (L=length, W=width). Define $\Phi = BS$, $\Phi_0 = h/e$, we obtain $N = 2 \times \frac{\Phi}{\Phi_0}$.

Remark Although $\Delta y_k \ll \Delta y$, $\langle \chi_{k_1}|\chi_{k_2}\rangle \neq 0$, $\langle k_1|k_2\rangle = 0$ in the x direction. So the whole wave function is orthogonal.

$\pi r_c^2 B = \pi\frac{\hbar}{m\omega_c}B = \frac{hm}{meB}B = h/e = \Phi_0, N = \frac{BS}{\Phi_0}$.

Remark For any B, the quantization of the cyclotron orbit ensures that the encircled flux is quantized.

1.5.3 $U \neq 0, B \neq 0$ (stripe subject to B)

$$\begin{aligned}
&[E_s + \frac{(\hbar k + eBy)^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega_0^2 y^2]\chi(y) = E\chi(y) \\
&[E_s + \frac{1}{2}m\omega_c^2(y + y_k)^2 + \frac{p_y^2}{2m} + \frac{1}{2}m\omega_0^2 y^2]\chi(y) = E\chi(y) \\
&[E_s + \frac{1}{2}m(\omega_c^2 + \omega_0^2)y^2 + \frac{p_y^2}{2m} + \frac{1}{2}m\omega_c^2 y^2 + m\omega_c^2 y_k y]\chi(y) = E\chi(y)
\end{aligned} \tag{1.100}$$

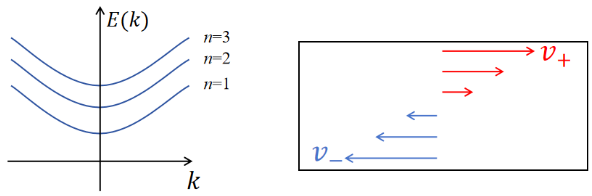
Define $\omega_0^2 + \omega_c^2 = \omega_{c_0}^2$,

$$\begin{aligned}
&[E_s + \frac{1}{2}m\omega_{c_0}^2 y^2 + \frac{p_y^2}{2m} + \frac{1}{2}m\omega_c^2 y^2 + m\omega_c^2 y_k y]\chi(y) = E\chi(y) \\
&[E_s + \frac{p_y^2}{2m} + \frac{1}{2}m\omega_c^2 y_k^2 + \frac{1}{2}m\omega_{c_0}^2(y^2 + \frac{2\omega_c^2}{\omega_{c_0}^2}y_k y + \frac{\omega_c^4}{\omega_{c_0}^4}y_k^2) - \frac{1}{2}m\frac{\omega_c^4}{\omega_{c_0}^4}y_k^2]\chi(y) = E\chi(y) \\
&[E_s + \frac{p_y^2}{2m} + \frac{1}{2}m\frac{\omega_c^2\omega_0^2}{\omega_{c_0}^2}y_k^2 + \frac{1}{2}m\omega_{c_0}^2(y + \frac{\omega_c^2}{\omega_{c_0}^2}y_k)^2]\chi(y) = E\chi(y)
\end{aligned} \tag{1.101}$$

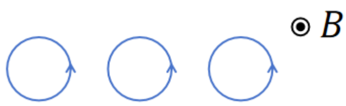
where $\chi_{n,k}(y) = u_n[q + \frac{\omega_c^2}{\omega_{c_0}^2} q_k]$, $q = \sqrt{m\omega_{c_0}/\hbar}\,y$, $q_k = \sqrt{m\omega_{c_0}/\hbar}\,y_k$,

$$E(n,k) = E_s + \frac{1}{2} m \frac{\omega_c^2 \omega_0^2}{\omega_{c_0}^2} y_k^2 + (n + \frac{1}{2})\hbar\omega_{c_0} = E_s + \frac{1}{2}\frac{\omega_0^2}{\omega_{c_0}^2}\frac{\hbar^2 k^2}{m} + (n + \frac{1}{2})\hbar\omega_{c_0} \tag{1.102}$$

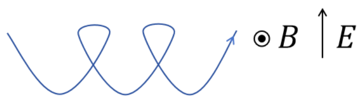
where $\omega_c y_k = \frac{\hbar k}{m}$. The velocity $v(n,k) = \frac{1}{\hbar}\frac{\partial E(n,k)}{\partial k} = \frac{\hbar k}{m}\frac{\omega_c^2}{\omega_{c_0}}$. Effect of magnetic field: $m \to m(1 + \frac{\omega_c^2}{\omega_{c_0}})$, electrons become fat. $y_k = \frac{\hbar k}{eB} \Rightarrow y_k = v(n,k)\frac{\omega_c + \omega_0^2}{\omega_c \omega_0^2}$, which means the transverse location of the wave function is proportional to its velocity.



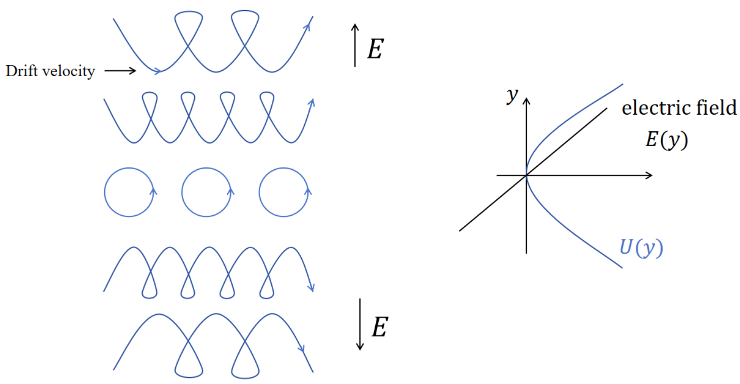
Classical picture: $B \neq 0, E = 0$:



$B \neq 0, E \neq 0$:



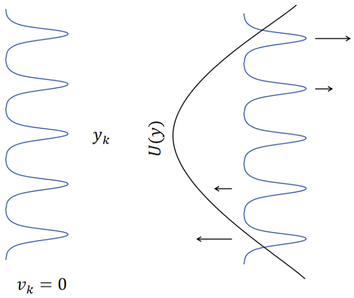
$U \propto y^2$:



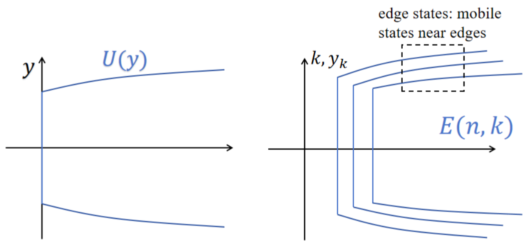
Introduce potential energy to each mode: $\int dy \langle \chi_{n,k}(y)|U(y)|\chi_{n,k}(y)\rangle = U_k$. For finite dispersion, $\frac{\partial E(n,k)}{\partial k} \sim \frac{U_k}{\partial k}$.

1.5.4 General scenario: topological edge states

Although this is obtained by the model with specific potential, the qualitative conclusion generally holds: edge states. To induce finite dispersion, $U(y)$ is finite only around the edge, with zero magnitude in the bulk.



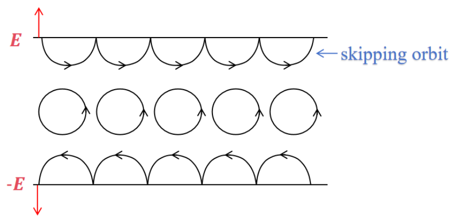
Transverse modes.



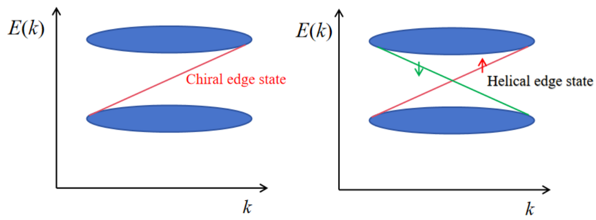
Question: *What is the physical meaning of "an edge"?*

Answer: *Confining potential.*

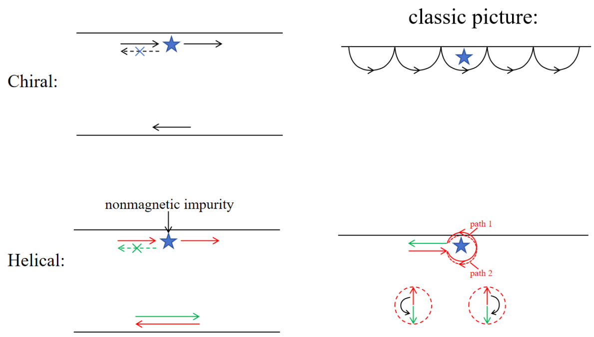
The edge states can be understood in two ways: (i) y-dependent $U(y)$ near the edges gives rise to finite dispersion. $v_k \sim \frac{\partial U_k}{\partial k} \sim \frac{\partial \langle \chi_{n,k}|U|\chi_{n,k}\rangle}{\partial k}$. (ii) Finite electric field $E_y = -\frac{\partial U(y)}{\partial y}$ at the edge gives rise to local Hall current.



Hall response is the intrinsic bulk property. (Bulk-Edge Correspondence→ PRB 25, 2185)



1.5.5 Suppression of backscattering



Chiral: right mover $|k\uparrow\rangle$, left mover $|k\downarrow\rangle$. Time reverse operator T: $T|k\uparrow\rangle = |-k\downarrow\rangle$, $T^2=-1$. $T|-k\downarrow\rangle = -|k\uparrow\rangle$. The nonmagnetic impurity: $TV(r)T^{-1}=V(r)$. T is an antiunitary operator: $\langle Tx|Ty\rangle = \langle y|x\rangle$, $T=i\sigma_y K = T^\dagger$, K: conjugate operator.

$$\begin{aligned}\langle -k\downarrow|V|k\uparrow\rangle &= -\langle k\uparrow|TVT|-k\downarrow\rangle = -(\langle k\uparrow|T^\dagger)V(T|-k\downarrow\rangle)\\ &= -(\langle k\uparrow|T^\dagger)(TV|-k\downarrow\rangle) = -\langle -k\downarrow|V|k\uparrow\rangle = 0\end{aligned} \tag{1.103}$$

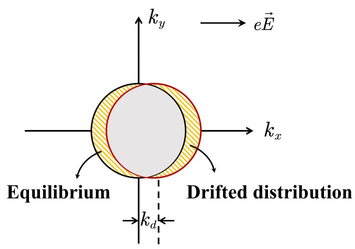
Helical: $\hat{R}_s(2\pi)=e^{i\pi}$. $a = r\hat{R}_s(\pi)+r\hat{R}_s(-\pi)$, $|a|^2 = 2|r|^2 + (|r|^2\hat{R}_s(2\pi)+c.c.) = 0$

1.6 Drift velocity or Fermi velocity

The current density $\vec{J}$ in a homogeneous conductor:

$$\vec{J} = en_s\vec{v}_d. \tag{1.104}$$

where n_s is the electron density, and the $\vec{v}_d$ is the drift velocity. In this picture, all electrons drift and contribute to the current. This picture contradicts that for degenerate electron gas, $k_BT \ll E_F - E_s$. Energy-resolved current measurements show that only electrons within a few k_By relative to quasi-Fermi energy F_n carry current. Conceptual simplification: For low temperatures, it is sufficient to understand the dynamics of electrons with energies close to the Fermi-energy.



$$[f(\vec{k})]_{E\neq 0} = [f(\vec{k}-\vec{k}_d)]_{E=0} \tag{1.105}$$

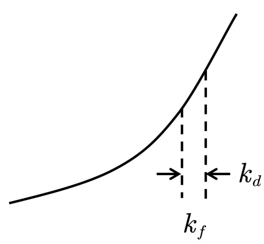
$$\frac{\hbar\vec{k}_d}{m} = \vec{k}_d = \frac{e\vec{E}\tau_m}{m} \Rightarrow \vec{k}_d = \frac{e\vec{E}\tau_m}{\hbar} \tag{1.106}$$

When $k_d \ll k_F$, nothing much happens for electrons deep inside the Fermi sea ($k \ll k_F$). This can be analyzed from two perspectives:

- Single-particle perspective: Electric field boosts all electrons by the drift velocity $\vec{v}_d$;
- Collective perspective: Electric field only moves a few electrons from $-k_F$ to k_F, a "pumping regime".

Rewrite the current density:

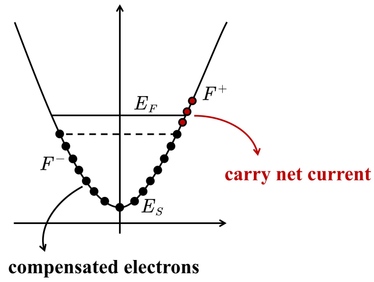
$$\vec{J} = en_s\vec{v}_d = e[n_s\frac{\vec{v}_d}{\vec{v}_F}]\vec{v}_F. \tag{1.107}$$



Current is carried by a small fraction of the total electrons ($n_s\frac{\vec{v}_d}{\vec{v}_F}$) which move with the Fermi velocity.

Remark The equivalent pictures arise because of Fermi-Dirac distribution. The current carried by electrons near E_F usually works for longitudinal current. The Hall current is usually understood by the entire Fermi sea. However, for topological transport, Hall current may also be interpreted by electrons at the Fermi level. $\oiint f(\vec{k})\Omega_{\vec{k}} d\vec{k}^2 = \oint_{E_F} \vec{A}(\vec{k}) \cdot d\vec{k}$, [see Haldane, PRL]

1.6.1 Quasi-Fermi level

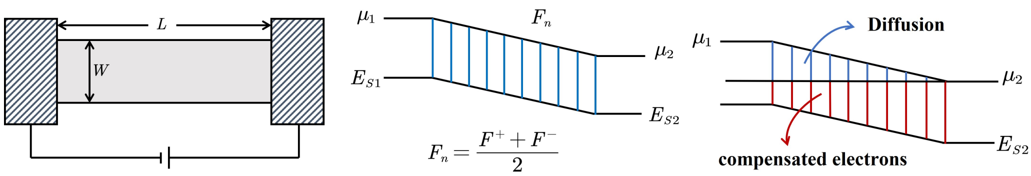


$$F^{\pm} \sim \frac{\hbar^2 (k_F \pm k_d)^2}{2m} \tag{1.108}$$

$$\Rightarrow F^+ - F^- \sim \frac{2\hbar^2 k_F k_d}{m} = 2eEv_F\tau_m = 2eEl \tag{1.109}$$

where l denotes the mean free path.

1.6.2 Einstein relation



Current density: $J = en_s\vec{v}_d$, drift current by all electron. $\vec{E} = \hat{x}V/L = \nabla E_s/|e|$, electric potential shifts the band. Homogeneous conductor: electron density is constant everywhere. Concentration gradient: $\nabla n = -N_s(\mu_1 - \mu_2)/L\hat{x}$. Diffusion current is given by: $\vec{J} = -eD\nabla n = eDN_s\frac{\mu_1-\mu_2}{L}\hat{x} = e^2DN_s\vec{E}$. Considering the chemical potential difference $\mu_1 - \mu_2 = eEL$, the conductivity is defined as $\sigma = e^2N_sD$.

1.6.3 Drift or diffusion, two different perspectives

(i) **Drift:** Consider entire sea of electrons, no concentration gradient, no diffusion. The current is then purely due to drift $\vec{J} = en_s\vec{v}_d$. so $\sigma = en_s\mu$, where n_s is the carrier density.

(ii) **Diffusion:** Focus on energy range $\mu_1 > E > \mu_2$. Finite concentration gradient. The current is then purely due to diffusion, we get:

$$\sigma = e^2 N_s D \tag{1.110}$$

$$\Rightarrow \frac{eD}{\mu} = \frac{n_s}{N_s} = E_F - E_s \tag{1.111}$$

$$\Rightarrow D = \frac{\mu}{e}(E_F - E_s) = \frac{\tau_m}{m}\frac{1}{2}mv_F^2 \tag{1.112}$$

$$\Rightarrow D = \frac{1}{2}v_F^2\tau_m \tag{1.113}$$

If $n_s \to 2n_s$, the following consequences ensue:

(i) $\sigma \to 2\sigma$, due to increase in electron density.

(ii) $E_F - E_s \to 2(E_F - E_s) \to \sigma \to 2\sigma$, due to increase in Fermi velocity v_F.

Conclusion

(i) More electrons that move.

(ii) The same number of electrons more faster.

Non-degenerate conductors: $\frac{eD}{\mu} = k_B T$.

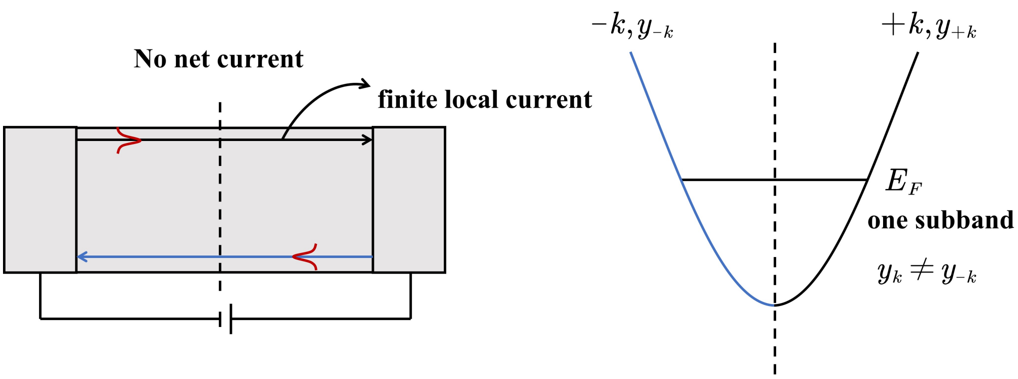
Question: *How does all the analysis change for Dirac Fermion?*

1.6.4 Zero temperature conductance is a Fermi surface property

$$\mu_1 + nk_BT > \varepsilon > \mu_2 + nk_BT. \tag{1.114}$$

$T \to 0$, then $\mu_1 \gtrsim \mu_2 \sim E_F$. To understand the conduction properties at low temperatures, it is sufficient to consider the diffusion of electrons right at the Fermi energy, without worrying the entire sea of electrons.

1.6.5 With magnetic field



It seems from the band shape that no difference from previous analysis. However, k is now y_k, meaning that the left- and right-movers are spatially separated. Therefore, the electrons below the Fermi energy. Although compensate each other for the overall current, not so for local current. That is to say, all electrons below E_F should be taken into account in the analysis of local current, which corresponding to conductivity as

$$\delta\vec{J} = \sigma\delta\vec{E}. \tag{1.115}$$

But is is still sufficient to consider electrons around Fermi energy in the analysis of the conductance. Electrons far below E_F, compensate each other in the overall current, summing up all transverse channels.

The statement ”zero temperature conductance is a Fermi surface properties” holds true for conductance is this scenario, rather than conductivity.

✍ **Exercise 1.2 (E.2.1, page 112)** In Section 2.1 we calculate the contact resistance when a narrow conductor with M modes is connected to two very wide contacts. If the number of modes in the contacts is not infinite, but some finite number, N, then the left-moving and right-moving carriers inside the contacts have different electrochemical potentials as shown in Fig. E.2.1 (page 112 of Datta's book). Show that the contact resistance taking this into account is given by

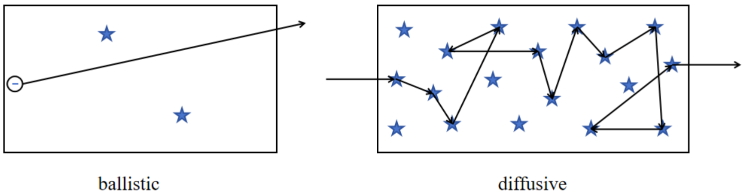
$$R_c = \frac{h}{2e^2}\left[\frac{1}{M} - \frac{1}{N}\right].$$

Assume reflectionless contacts as in the text. For futher discussions on the nature of the contact resistance at different types of interfaces see R. Landauer (1989), *J.Phys. Cond. Matter*, **1**, 8099 and M. C. Payne (1989), *J. Phys. Cond. Matter*, **1**, 4931.

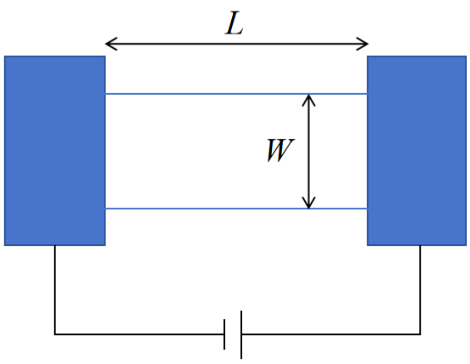
Chapter 2 Landauer-Büttiker Method

2.1 Resistance of a ballistic conductor

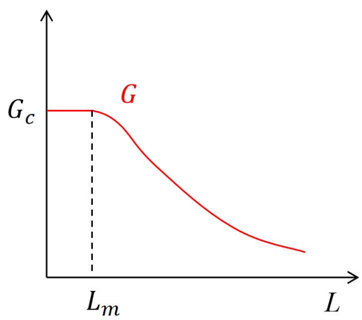
2.1.1 Ballistic v.s. diffusive



ballistic: propagation without scattering, no impurity or weak effectiveness of scattering (topological edge state).

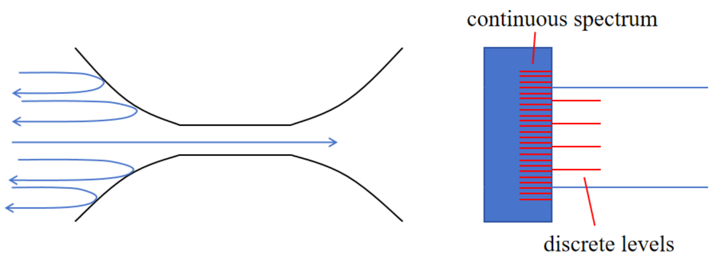


Large conductors: ohmic scaling $G = \sigma W/L$. $L \to 0, G \to \infty$, unphysical. Experiment: $L \gg L_m, L \to 0, G \to G_c$.



2.1.2 Contact resistance, concept

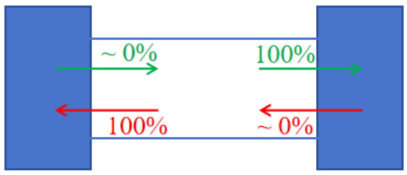
where comes the resistance for a ballistic conductor? G_c^{-1} is referred to as contact resistance. Contact: infinitely many transverse modes. Conductor: a few transverse modes. Most incident electrons are reflected. "From sea to river".



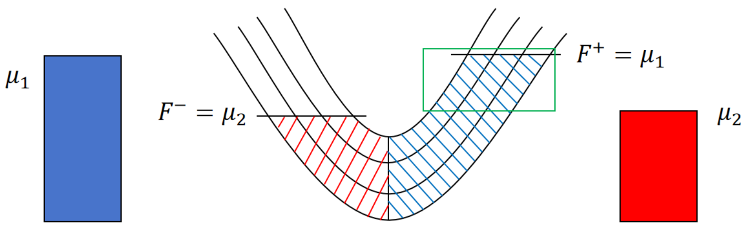
The contact cannot be identical to the conductor. The contacts should be infinitely large such that electrons inside can be regarded as in equilibrium, the tiny current flowing inside the conductor will not affect such equilibrium. Therefore, y=the chemical potentials in the contacts are well defined and the voltage drop occurs entirely within the conductor.

2.1.3 Reflections contacts

Reflection is negligible when electrons transport from the conductor to the contacts.



Without relaxation and scattering within the conductor. Right-moving electrons possess the same distribution as that in the left contact. Left-moving electrons possess the same distribution as that in the right contact.



At low temperatures, current is due to the green part.

2.1.4 Calculating the current

For the N-th mode dispersion $E(N,k)$, $\varepsilon_N = E(N,0)$, band edge. Number of modes for a given energy E: $M(E) = \sum_N \theta(E - \varepsilon_N)$. For any mode, $+k$ states occupied according to distribution function $f^+(E)$. Consider the current, $dq = evndt \Rightarrow I = evn, n = 1/L$.

$$I^+ = \frac{e}{L}\sum_k v_k f^+(E) = \frac{e}{L}\sum_k \frac{1}{\hbar}\frac{\partial E}{\partial k} f^+(E) \tag{2.1}$$

$\sum_k \to 2 \times \frac{L}{2\pi}\int dk \Rightarrow$

$$I^+ = \frac{2e}{L}\frac{L}{2\pi}\int_0^\infty \frac{dk}{\hbar}\frac{\partial E}{\partial k} f^+(E) = \frac{2e}{h}\int_\varepsilon^\infty f^+(E)dE \tag{2.2}$$

Multiple modes:

$$I^+_{total} = \sum_N I^+(N) = \sum_N \frac{2e}{h}\int_\varepsilon^\infty f^+(E)dE = \frac{2e}{h}\int_{-\infty}^\infty f^+(E)M(E)dE \tag{2.3}$$

Remark this relation holds for any kind of dispersion, the main task becomes counting numbers of transverse modes occupied. The reason is that larger velocities correspond to smaller DOS.

The current carried per mode per unit energy by an occupied state: $2e/h \simeq 80$nA/meV.

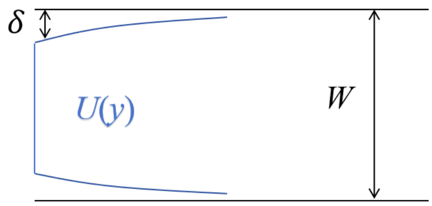
2.1.5 Contact resistance, evaluation

$$I = I^+ - I^- = \frac{2e}{h}\int_{-\infty}^\infty [f^+(E) - f^-(E)]M(E)dE \tag{2.4}$$

where $f^+(E)$ is the Fermi distribution of left contact, and $f^-(E)$ is the Fermi distribution of right contact. Consider zero temperature, $f^+(E) = \theta(\mu_1 - E)$, $f^-(E) = \theta(\mu_2 - E)$. Assume $\mu_1 - \mu_2 \ll \Delta\varepsilon$ (energy shift between different transverse modes), then both μ_1 and μ_2 cross M modes.

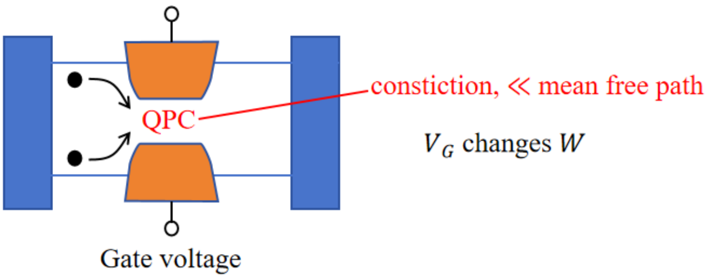
$$I = \frac{2e}{h}\int_{-\infty}^\infty \theta(\mu_1 - E)\theta(E - \mu_2)M(E)dE = \frac{2e}{h}M(\mu_1 - \mu_2) \tag{2.5}$$

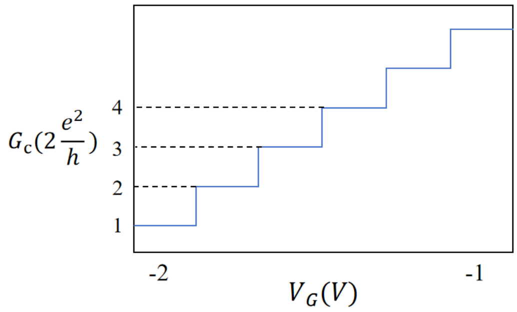
where $\mu_1 - \mu_2 = eV$, $I = \frac{2e^2}{h}MV \Rightarrow G_c = \frac{\partial I}{\partial V}$ (differential conductance) $= \frac{I}{V}$ (conductance) $= \frac{2e^2}{h}M$. The contact resistance (resistance of ballistic conductor): $G_c^{-1} = \frac{h}{2e^2}\frac{1}{M} \simeq \frac{12.9\text{k}}{M}$, where the numerator is the single-mode resistance, and the denominator is parallel resistors composed by different modes.



Wide conductors and scaling with W: $U(y)$ changes in the scale δ at the boundary, which satisfy $\delta \gg W$. To count the transverse modes, we neglect the boundary details and use the periodic boundary conditions. The transverse modes are then marked with k_y. $\Delta y = \frac{2\pi}{W}$ (Born-von Karmen boundary condition), $E_F = \frac{\hbar^2 k_F^2}{2m}$, $-k_F < k_y < k_F$, the channels all cross E_F. Plane waves replace standing waves composed of k_y. $M(E_F)$ =Int$[\frac{\Delta k_F}{\Delta k_y}]$ =Int$[\frac{k_F W}{\pi}]$ =Int$[\frac{W}{\lambda_{F/2}}]$, where λ_F is the Fermi wave length. Consider $\lambda_F = 30$nm, $W = 15\mu$m (FET) $\Rightarrow M \simeq 1000$. $G_c^{-1} \simeq 12.5\Omega$.

2.1.6 Experiment on quantum point contacts (QPC)

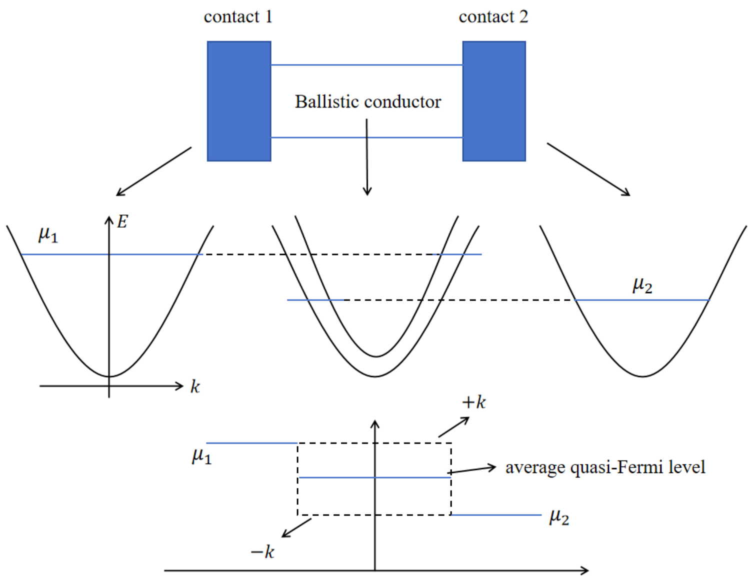




Quantized (differential) conductance

Metal: small λ_F, large M, $V_G \to \Delta W \to \Delta M \gg 1$. Semiconductor: large λ_F, small M, quantization, $\Delta W \to \Delta M \sim 1$.

2.1.7 where is the voltage drop?



For small current, the chemical potential is near equal for $\pm k$ states in contacts, with huge difference between quasi-Fermi level in the conductor, $F^+(=\mu_1) \neq F^-(=\mu_2)$. Define the average quasi-Fermi level,

$F = \frac{1}{2}(F^+ + F^-) = \frac{1}{2}(\mu_1 + \mu_2)$. Where the voltage drops, where the resistance is located. The voltage drops are equal at two interfaces, indicating that the resistance is located at the interfaces, consistent with the “contact resistance”.

2.2 Landauer Formula

Mesoscopic v.s. Macroscopic (ohm’s law $G = \sigma W/L$).

(1) Contact resistance independent of L.

(2) $G \propto M$, M does not $\propto W$, exhibiting discrete steps.

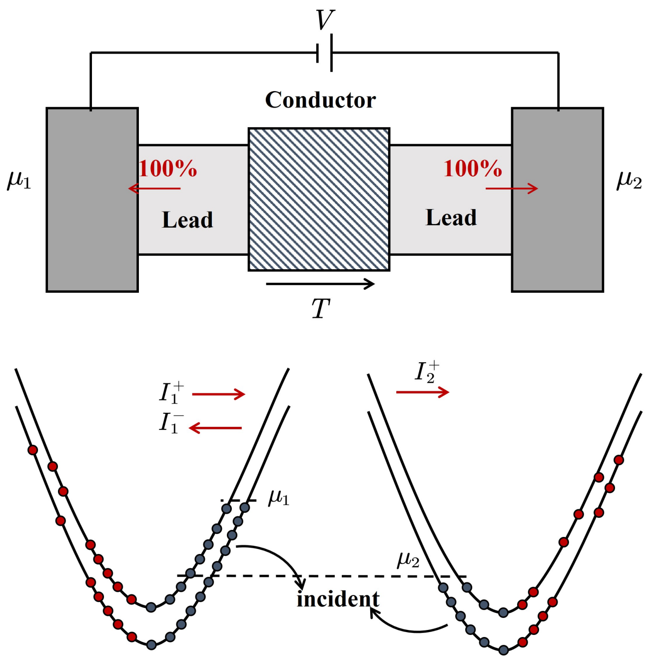
- **Landauer Formula:**

$$G = \frac{2e^2}{h} MT, \tag{2.6}$$

where T represents the average transmission probability, with $T = 1$ indicating a ballistic conductor.

- **Lead:** ballistic conductor with M transverse modes.

The contacts are reflectionless, so that the incident electrons ($\pm k$ states in lead 1 and 2) possess the same distributions as those in the corresponding contacts.



Remark The leads with proper distribution functions for the incident states contain the full information that is necessary for the calculation of the transport properties, effectively describing the physical roles of both the leads and contacts. The electron distribution below μ_2 is unaffected by scattering up to an over all $U(1)$ phase.

Zero temperature. influx of electrons from lead 1:

$$I_1^+ = \frac{2e}{h} M[\mu_1 - \mu_2] \tag{2.7}$$

Outflux from lead 2:

$$I_2^+ = \frac{2e}{h} M(1-T)[\mu_1 - \mu_2] \tag{2.8}$$

Net current:

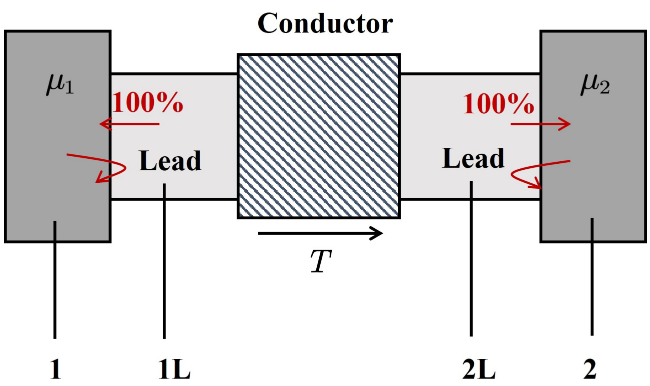
$$I = I_2^+ = I_1^+ - I_1^- = \frac{2e}{h} MT[\mu_1 - \mu_2] \tag{2.9}$$

$$\Rightarrow G = \frac{I}{V} = \frac{2e^2}{h} MT \tag{2.10}$$

where T represents the mean transmission probability, and $T = 1$ indicates a ballistic conductor. We could view the Landauer formula as a mesoscopic version of the Einstein relation:

$$\sigma = e^2 N_s D \qquad \sigma \to G, N_s \to M, D \to T. \tag{2.11}$$

2.2.1 Should we include the contacts?



Question: *Calculate transmission between 1, 2, or 1L, 2L?*

Between 1, 2, we should include the number of modes M_w in the wide contacts. Due to the restricted structure is the central region, average transmission probability for a single mode is very small.

For a ballistic conductor, whether $T_w \sim M/M_w$ such that $G = \frac{2e^2}{h} M_w T_w = \frac{2e^2}{h} M$ is hard to verify.

Although $G = \frac{2e^2}{h} MT$ measure the conductance between 1, 2, we just need to evaluate the quantity MT between 1L, 2L, rather than that between 1, 2. It saves a lot of work but leads to the same answers.

Justifications:

(1) Contacts are in equilibrium, with $F^+ \simeq F^-$.

(2) Incident electrons inherit the distributions of the corresponding contacts.

(3) Distributions of incoming electrons plus transmission are sufficient for the derivation of the Landauer formula for reflectionless contacts.

(4) Ultimately tested by experiment.

Remark Contacts provide distributions inherited by incoming electrons in the leads, while conductor provides scattering. In this way, we can forget the contacts.

2.2.2 Ohm's law

How can we reobtain the Ohm's law from Landauer formula as the conductor's size becomes large.

Wide conductor:

$$M \sim k_F W/\pi \tag{2.12}$$

$$G = \frac{2e^2}{h}\frac{k_F W}{\pi}T \tag{2.13}$$

$$= \frac{2e^2}{h}\frac{\hbar k_F}{m}\frac{m}{\hbar}\frac{W}{\pi}T = \frac{e^2}{\pi\hbar}v_F\frac{m}{\hbar}\frac{W}{\pi}T = e^2 W N_s v_F T/\pi \tag{2.14}$$

where we have utilized the expression $N_s = m/\pi\hbar^2$.

The transmission probability (classical) through a conductor of length L.

$$T = \frac{L_0}{L + L_0} \tag{2.15}$$

L_0, which denotes the characteristic length, is approximately equal to the mean free path. $L \to 0$, $T \to 1$. We introduce the expression for T, leading to

$$G = \frac{W}{L + L_0}e^2 N_s(v_F L_0/\pi) \tag{2.16}$$

Recall Einstein's relation for degenerate conductors, given as $\sigma = e^2 N_s D$, where $D = \frac{1}{2}v_F^2\tau_m$, so

$$G = \frac{\sigma W}{L + L_0} \Rightarrow G^{-1} = \frac{L + L_0}{\sigma W} \quad \text{(resistance)} \tag{2.17}$$

we can rewrite the resistance as:

$$G^{-1} = G_s^{-1} + G_c^{-1} \tag{2.18}$$

where $G_s^{-1} = \frac{L}{\sigma W}$ is the actual resistance, obey the Ohm's law, and the $G_c^{-1} = \frac{L_0}{\sigma W}$ is the contact resistance.

Proof of $T(L) = L_0/(L + L_0)$ in the classical regime:

Is $T_{12} = T_1 T_2$? Certainly not! If that were the case, we would have:

$$T_{12} = T_1 T_2 \tag{2.19}$$

$$\Rightarrow T(x_1 + x_2) = T(x_1)T(x_2) \tag{2.20}$$

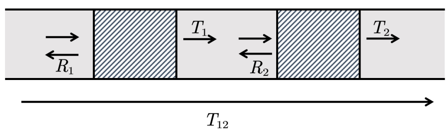
$$\Rightarrow \log T(x_1 + x_2) = \log T(x_1) + \log T(x_2) \tag{2.21}$$

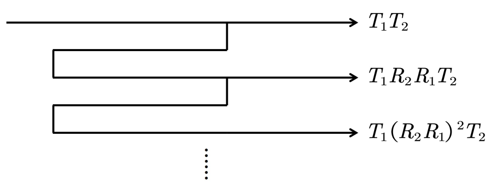
We define the function $f(x)$ as $\log T(x)$, and thus we have:

$$f(x) = C \cdot x \Rightarrow T(x) = e^{cx} \tag{2.22}$$

$$\Rightarrow T(x_1 + x_2) = T(x_1)T(x_2) \tag{2.23}$$

$$\Rightarrow T(x) \sim e^{-x}, T(L) \sim e^{-L} \tag{2.24}$$





Correct method to calculate resistance:

$$T_{12} = T_1\left(1 + R_1R_2 + R_1^2R_2^2 + ...\right)T_2 = \frac{T_1T_2}{1 - R_1R_2} \tag{2.25}$$

$$\Rightarrow \frac{1}{T_{12}} = \frac{1 - (1 - T_1)(1 - T_2)}{T_1T_2} = \frac{T_1 + T_2 - T_1T_2}{T_1T_2} = \frac{1}{T_1} + \frac{1}{T_2} - 1 \tag{2.26}$$

$$\Rightarrow \frac{1 - T_{12}}{T_{12}} = \frac{1 - T_1}{T_1} + \frac{1 - T_2}{T_2} \tag{2.27}$$

We see that $\frac{1-T_1}{T_1}$ shows an additive property. So for N

identical scatters in series, each having a transmission probability T, we have:

$$\frac{1-T(N)}{T(N)} = N\frac{1-T}{T} \Rightarrow T(N) = \frac{T}{N(1-T)+T} \tag{2.28}$$

The number of scatters $N = \nu \cdot L$, ν linear density of scatters:

$$T(N) = \frac{T}{\nu L(1-T)+T} = \frac{T/\nu(1-T)}{L+T/\nu(1-T)} = \frac{L_0}{L+L_0} \tag{2.29}$$

where $L_0 = \frac{T}{\nu(1-T)}$ is order of MFP. To see this, we have $1 - T\nu l \sim 1$, so that $l \sim \frac{1}{\nu(1-T)} \sim L_0$.

The quantity $(1-T)/T$ has an additive property actually suggests that the actual resistance of the conductor satisfies the Ohm's Law.

$$G^{-1} = \frac{h}{2e^2M}\frac{1}{T} = \frac{h}{2e^2M} + \frac{h}{2e^2M}\frac{1-T}{T} \tag{2.30}$$

$$= G_c^{-1} + G_s^{-1} \tag{2.31}$$

$$G_s^{-1} = \frac{h}{2e^2M}\sum_i \frac{1-T_i}{T_i} = \sum_i G_{si}^{-1} \tag{2.32}$$

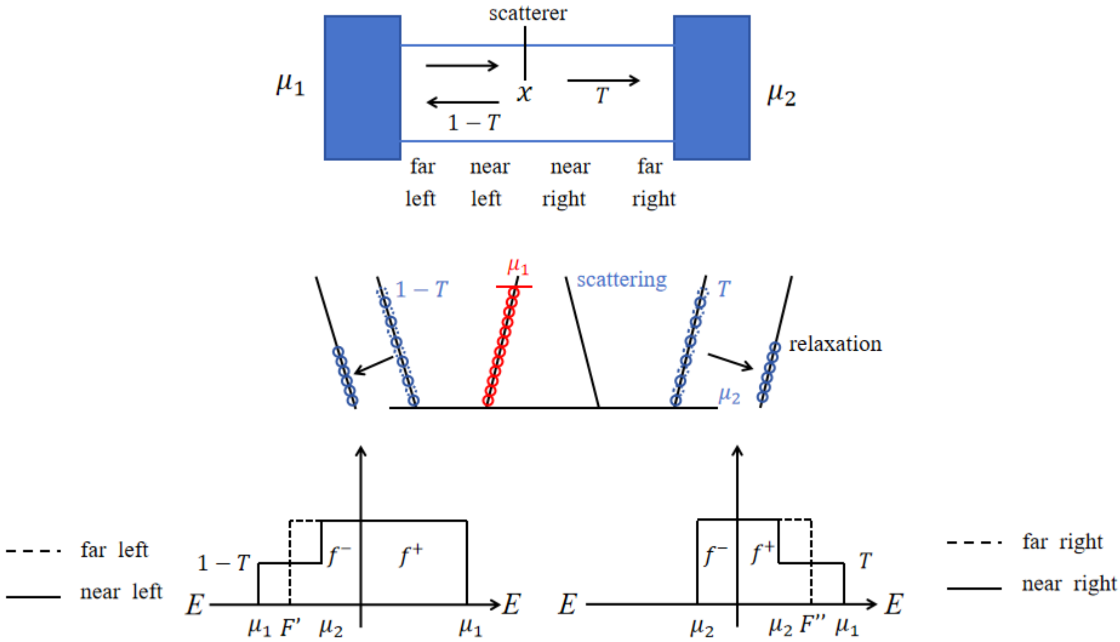
Remark Quantum coherence effect is not involved, which is the main focus of this lecture. As the quantum interference is taken into account Ohm's law fails for G_s^{-1}. At the same time, the multiple scattering picture holds even for quantum regime, as the phase coherence correction is considered.

2.3 Where is the resistance

what's the nature and meaning of resistance on a microscopic scale? Drude model gives some pictures, but the microscopic picture is averaged out to give the results on a macroscopic scale. Consider a conductor with M modes with one scatterer with T. $G^{-1} = G_c^{-1} + G_s^{-1}, G_c^{-1} = \frac{h}{2e^2M}, G_s^{-1} = \frac{h}{2e^2M}\frac{1-T}{T}$ (This "Ohm's" law holds even when G_s^{-1} involves quantum coherence). The scatterer resistance G_s^{-1} is determined entirely by the transmission probability T. But there are several questions associated with various manifestations of the resistance that remain. (1) Can we associate the resistance just with the scatterer? (2) What about the potential drop (I/G_s) associated with this resistance? Does it occur right across the scatterer? (3) What happens to the Joule heat (I^2/G_s) associated with this resistance? Is it dissipated at the scatterer? (4) The scatterer could be rigid and elastic having no internal DoF to dissipate energy. In that case, the heat must be dissipated elsewhere. But where?

2.3.1 Energy distribution of electrons

when a bias is applied, electrons are injected into the leads, inheriting the distribution of the contacts. Then electrons are scattered, the outgoing electrons are in non-equilibrium states, which are determined by scattering and then undergo relaxation to equilibrium far from the scatterer.

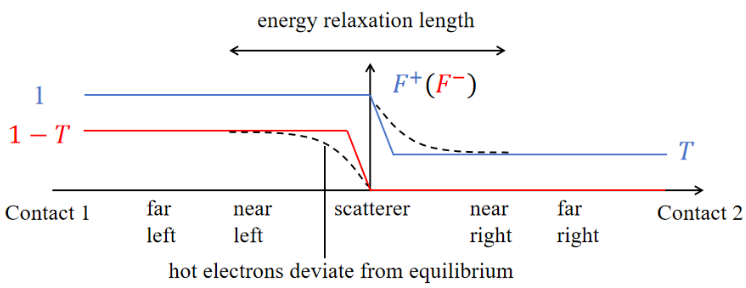


$f^{\pm}(E)$ are distribution functions for $\pm k$ states.

At low temperatures, $f^+(E) \simeq \theta(\mu_1 - E)$ (left of scatterer, μ is the electrochemical potential). Incident electrons are in equilibrium, no relaxation can occur before scattering. Similarly, $f^-(E) \simeq \theta(\mu_2 - E)$ for the right of scatterer. Scattering results in non-equilibrium outgoing states. $f^+(E) \simeq \theta(\mu_2 - E) + T[\theta(\mu_1 - E) - \theta(\mu_2 - E)]$ for near left, $f^-(E) \simeq \theta(\mu_1 - E) + T[\theta(\mu_2 - E) - \theta(\mu_1 - E)]$ for near right. These distributions are highly non-equilibrium and are only valid very near the scatterer. After propagating through a few energy relaxation length away from the scatterer, the electrons will settle down to lower energies and a Fermi distribution will be established again. $f^+(E) \simeq \theta(F'' - E)$ for far right and $f^-(E) \simeq \theta(F' - E)$ for far left. The new electrochemical potentials F', F'' are determined by the conservation of electron number. $F'' = \mu_2 + T(\mu_1 - \mu_2)$, $F' = \mu_2 + (1 - T)(\mu_1 - \mu_2)$.

Remark (1) we have assumed that the energy relaxation processes occur within the $+k$ or $-k$ branch, but not in between. There is no momentum relaxation in such processes. As such, the resistance (momentum relaxation) and energy dissipation are separated. This is a simplified procedure to deal with the problem. Otherwise, additional resistance appears along with energy dissipation. (2) The analysis above has implicity used that the DOS is a constant, independent on energy for 2D electron gas or within a small energy interval.

2.3.2 spatial variation of the electrochemical potential

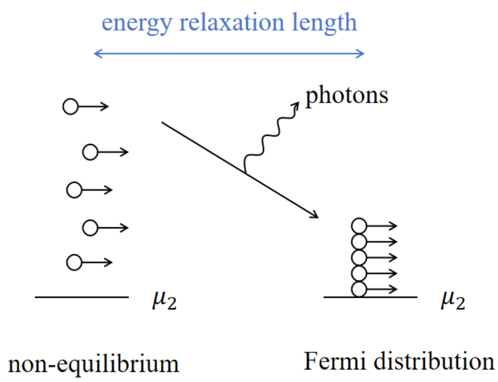


If we define the electrochemical potential even for the non-equilibrium regions such that it gives the right electron number using equilibrium distribution function, then we have for the $\pm k$ states: $F^+ = \mu_1$ (left)= $F'' = \mu_2 + T(\mu_1 - \mu_2)$ (right). Similarly, for the $-k$ states, $F^- = \mu_2$ (right)= $F' = \mu_2 + (1-T)(\mu_1 - \mu_2)$ (left). Define the normalized potentials $\mu^\pm$ of $F^\pm$ by setting $\mu_2 = 0, \mu_1 = 1$. one obtains $\mu^+ = 1$ (left), $\mu^+ = T$ (right), $\mu^+ = 1 - T$ (left), $\mu^- = 0$ (right). The normalized potential drops across the scatterer is equal to $1-T$ for both $\pm k$ states. The actual potential drop is then $eV_s = (1-T)(\mu_1 - \mu_2)$. The total voltage drop between 1,2 in the contacts is $\mu_1 - \mu_2$. Therefore, the rest of the bias $T(\mu_1 - \mu_2)$ is dropped at the interfaces with the contacts. Note that the current is $I = \frac{2e}{h} MT(\mu_1 - \mu_2)$, the contact resistance is $G_c^{-1} = \frac{h}{2e^2 M} \Rightarrow eV_c = eIG_c^{-1} = T(\mu_1 - \mu_2)$.

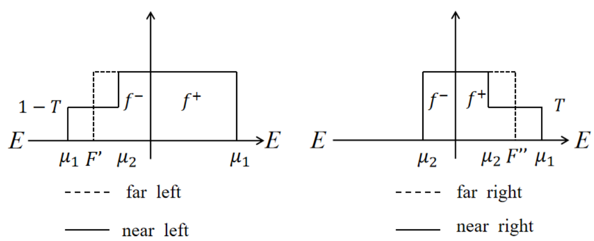
Remark One physical effect associated with the resistance is the voltage drop, $V = IR_s$. Using the assumption of $F^\pm(\mu^\pm)$ above, the voltage drop occurs spatially located at the scatterer, seemingly indicating $R_s = G_s^{-1}$ is also spatially located at the scatterer. But the resistance has different manifestations, it becomes subtle as G_s^{-1} is defined by these physical manifestations.

2.3.3 where is the heat dissipated?

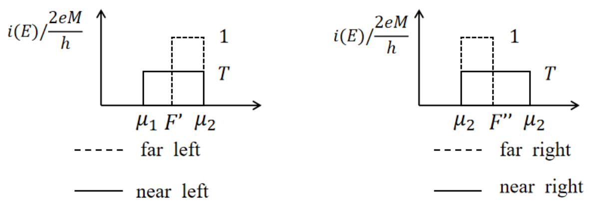
If G_s^{-1} is manifested through Joule heat I^2/G_s, then the property of G_s^{-1} is associated with spatial energy dissipation. Assuming rigid scatterer, the heat dissipation must occur elsewhere.



Consider energy conservation: $\partial U(z)/\partial t + \nabla \cdot \vec{j}_U + \rho_D(z) = 0$, where U is the energy of electron, $\vec{j}_U$ is the energy current, ρ_D is the dissipation. For stationary states, $\partial U(z)/\partial t = 0$, $\rho_D = -\nabla \cdot \vec{j}_U = -\frac{\partial I_U}{\partial z}$, $I_U = \frac{1}{e} \int Ei(E)dE$, $i(E)$ is the energy distribution of the current, $\frac{1}{e} i(E)dE$ denotes the current of carriers between $[E, E+dE]$. Charge current: $I = \int i(E)dE$ =constant. Define an average energy U of the current, $U = \frac{\int Ei(E)dE}{\int i(E)dE} = \frac{eI_U}{I} \Rightarrow \rho_D = -\frac{I}{e}\frac{dU}{dz}$. Current per unit energy: $i(E) = \frac{2eM}{h}[f^+(E) - f^-(E)]dE$. Again, $f^\pm$ is the distribution function for $\pm k$ states.



Energy distribution of particle number $f^\pm(E)$



Energy distribution of current $i(E)$, contributed by both left and right movers.

The average energy of the current (note that the discussion of energy is associated with the net current, since only this part of energy will dissipate):

$$U = \begin{cases} (F' + \mu_1)/2 & \text{(far left)}\sim 1 - \frac{T}{2} \\ (\mu_1 + \mu_2)/2 & \text{(near left and near right)}\sim \frac{1}{2} \\ (F'' + \mu_2)/2 & \text{(far right)}\sim \frac{T}{2} \end{cases}$$

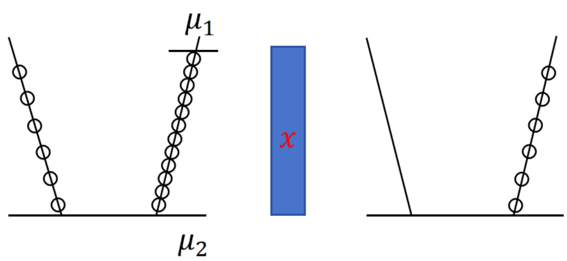
$U = \frac{eI_U}{I}$, so that for $T \neq 1$, both I_U and I are reduced by scattering by the same factor and $U = (\mu_1 + \mu_2)/2$ around the scatterer is independent on T. However, F', F'' rely on T.

while the electrochemical potential drops sharply across the scatterer, the average energy of the current changes slowly over an energy relaxation length which is the distance required to dissipate the Joule heat associated with G_s^{-1}. If we consider G_s^{-1} related to Joule heat, G_s^{-1} is not localized at the scatterer.

Remark G_s^{-1} has different manifestations: momentum relaxation, voltage drop, energy dissipation. We cannot discuss G_s^{-1} without talking about any of these effects. We did not touch the inelastic processes that dissipate current energy, just assuming they are inevitably present.

2.3.4 Resistivity dipoles

The quasi-Fermi energy F_n drops sharply at the scatterer.

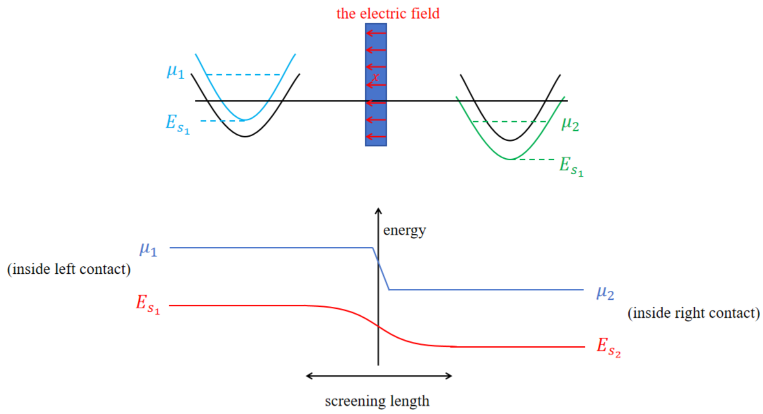


Energy distribution of particle number $f^{\pm}(E)$

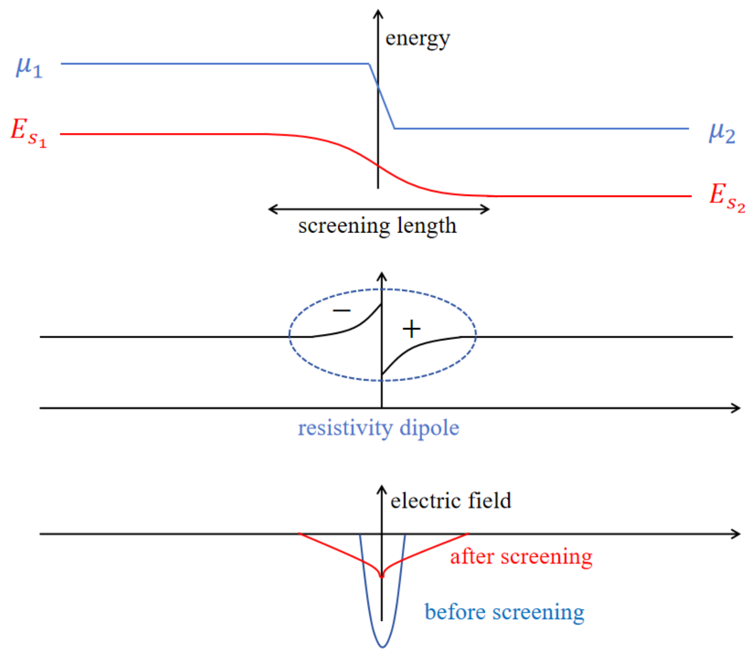
Since the quasi-Fermi energy is a measure of the electron number, and only a fraction (T) of electrons can cross the scatterer. Such a sharp change of electron number in space creates a strong local electric field. This effect appears only around the scatterer within the scale of screening length. Deeply inside the leads (contacts), the electron density should not change. This follows from the lesson of the screening effect in a metal. If there is a local charge therein, only electrons nearby will be driven to form the screening cloud. While other electrons far away from the local charge cannot even feel its existence. Therefore, the bottom of the band E_s follows the change of the electrochemical potential in space. In particular, $\mu_1 - E_{s_1} = \mu_2 - E_{s_2}$ ensures the same electron density deep inside the leads, which should be the asymptotic behavior of the actual situation.

When we impose a bias, what do we actually do?

Deep inside the leads, the electron density is unchanged, and so both μ_i, E_{s_i} change to ensure constant $\mu_i - E_{s_i}$. However, care should be taken near the scatterer, where charge imbalance occurs, which causes local field to be screened. Such a screening takes place in the the scale of screening length ($\sim$ a few angstroms in typical semiconductors), thus softens both the local field as well as change imbalance caused by scattering. Accordingly, E_{s_i} changes smoothly in space following the electrostatic potential. The latter is determined by the originally imbalanced charge due to scattering as well as the screening charge.



The physical effect involves the following steps: (1) Abrupt change electron density across the scatterer, with strong local electric field $\vec{E}_0$, (2) $\vec{E}_0$ drives free electrons for screening. (3) Both electron density and $\vec{E}$ field become smooth in space. The electron density $n_s = N_s(F_n - E_s) \Rightarrow \delta n_s = N_s(\delta F_n - \delta E_s)$. In the region of scatterer, $\delta n_s \neq 0$, $\delta F_n \neq \delta E_s$.



Remark This is a mesoscopic version of what happens on a macroscopic scale, where a low conductivity material. It also indicates that even a homogeneous conductor with a uniform conductivity is reallyu extremely inhomogeneous on a mesoscopic scale.

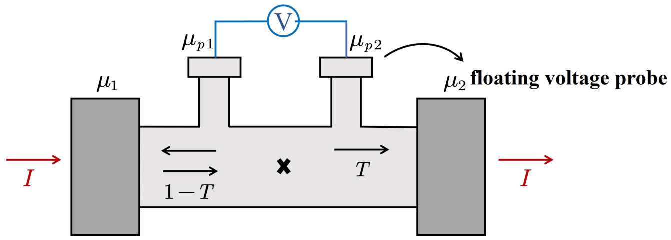
2.3.5 Screening length

Poisson equation for the electric potential $\nabla^2 V = -\frac{e^2(\delta n_s)}{\varepsilon d}$, where ε is the dielectric constant, d is the thickness of 2D system. (Note: δn_s is the area density, the system is in fact 3D.) $\delta E_s = \delta V \Rightarrow \nabla^2(\delta E_s) = -\frac{e^2(\delta n_s)}{\varepsilon d}$, $\nabla^2(\delta E_s) = -\frac{e^2 N_s(\delta F_n - \delta E_s)}{\varepsilon d} = -\beta^2(\delta F_n - \delta E_s), \beta = \sqrt{\frac{e^2 N_s}{\varepsilon d}} \Rightarrow (\nabla^2 - \beta^2)\delta E_s = -\beta^2 \delta F_n$, where β^{-1} is the screening length.

Remark E_s follows the electric potential, n_s is determined by the quasi-Fermi energy F_n.

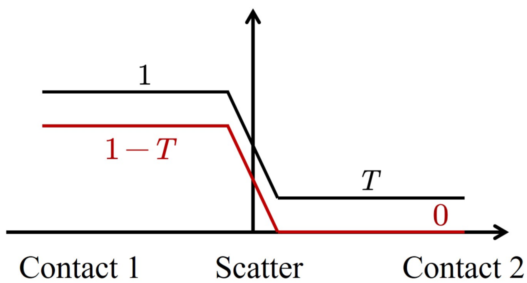
2.4 What does a voltage prob measure

Voltage probe: sense the local electrochemical potential (or quasi-Fermi energy)



Four-probe Hall bridge.

For macroscopic setups, there is no ambiguity for the electrochemical potential. However, for mesoscopic setups, it is highly nontrivial what a voltage probe actually measure. The electrochemical potentials for the $\pm k$ states differ from each other, and the signature of the voltage probe strongly relies on the details of the contacts between the sample and the probes.



If we assume that the probes will measure the local electrochemical potential of either $+k$ or $-k$ states, or some specific combination of the two, such as $\alpha\mu_{+k} + (1-\alpha)\mu_{-k}$ then we have:

$$\begin{cases} \mu_{p_1} &= \alpha\mu_1 + (1-\alpha)[\mu_2 + (1-T)(\mu_1 - \mu_2)] \\ \mu_{p_2} &= \alpha[\mu_2 + T(\mu_1 - \mu_2)] + (1-\alpha)\mu_2 \end{cases} \tag{2.33}$$

so

$$eV = \mu_{p_1} - \mu_{p_2} = \alpha[\mu_1 - \mu_2 - T(\mu_1 - \mu_2)] + (1-\alpha)[\mu_2 + (1-T)(\mu_1 - \mu_2) - \mu_2] \tag{2.34}$$

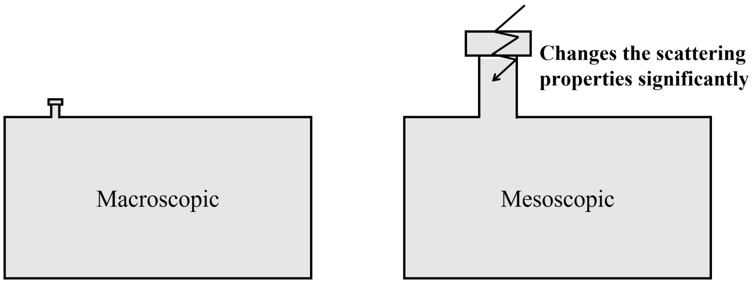
$$= \alpha(1-T)(\mu_1 - \mu_2) + (1-\alpha)(1-T)(\mu_1 - \mu_2) \tag{2.35}$$

$$= (1-T)\Delta\mu \tag{2.36}$$

where $\Delta\mu \equiv \mu_1 - \mu_2$. The expression for the current is $I = \frac{2e}{h} MT\Delta\mu$, leading to the four-terminal resistance $R_{4t} = \frac{V}{I} = \frac{h}{2e^2M}(\frac{1}{T} - 1) = R - R_c$, which is contributed by scattering expected result.

Three separate problems:

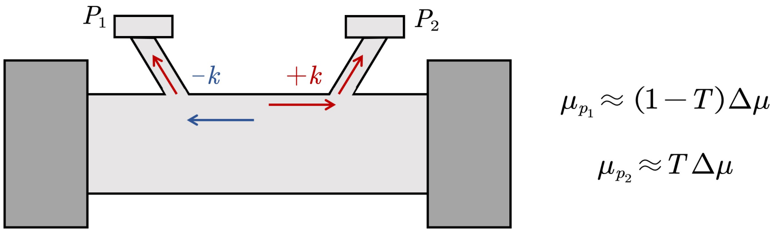
(1) Invasive mesoscopic probes



A practical rather than a fundamental problem. (Weakly coupled STM may solve this problem, very weak effect to mesoscopic conductor.)

(2) Non-identical mesoscopic probes

Different voltage probes could couple differently to the $+k$ and $-k$ states. In the limiting case shown in the following figure



$$R = \frac{(\mu_{p_1} - \mu_{p_2})/e}{I} = \frac{h}{2e^2M}\frac{1-2T}{T} \quad (R < 0 \quad \text{for} \quad T > 0.5) \tag{2.37}$$

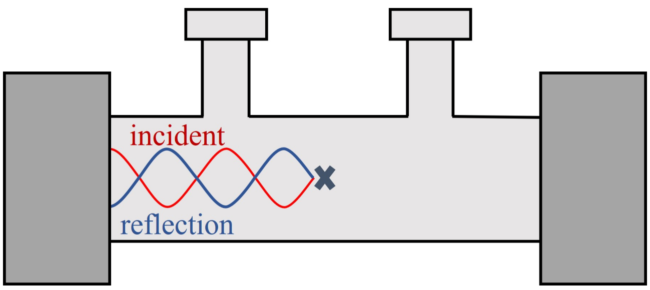
$$\mu_{p_1} - \mu_{p_2} \in [1-2T, 1]\Delta\mu \tag{2.38}$$

$$\Rightarrow R_{4t} = \frac{h}{2e^2M}\frac{1}{T}[1-2T, 1] \tag{2.39}$$

and for $L \gg l, T \ll 1, R_{4t} \simeq \frac{h}{2e^2M}\frac{1}{T} \gg R_c$.

(3) Quantum interference effects

$R_{4t} = \frac{h}{2e^2M}\frac{1-T}{T}$ can give correct description only if such interference effects are either absent (short phase-relaxation length) or carefully eliminated (averaging measurements over a wavelength or using "directional couplers") to couple the probes so that they see only $+k$ or $-k$ states.



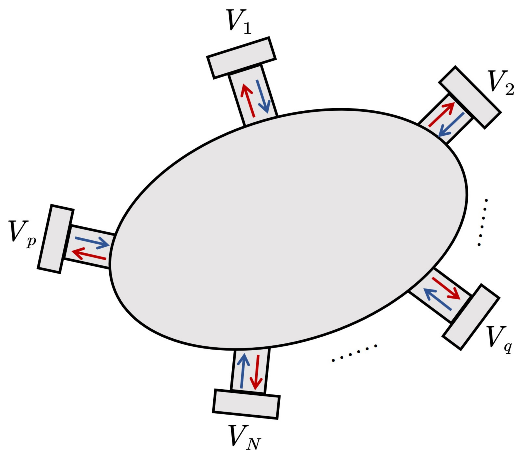
Conclusion *Adding contacts to the system (even voltage probes) inevitably changes the system and results of measurements involving other contacts. This is an example of the fact that in a quantum world any measurement inevitably affects the objects being measured.*

2.4.1 Büttiker formula

Büttiker formula:

(i) Treat current and voltage probes on an equal footing.

(ii) Completely bypass any questions regarding the internal states of the conductor.



Extend the two-terminal linear response formula

$$I = \frac{2e}{h}\bar{T}[\mu_1 - \mu_2] = I_1 = \frac{2e}{h}(\bar{T}_{21}\mu_1 - \bar{T}_{12}\mu_2) \tag{2.40}$$

to multi-terminal regime:

$$I_p = \frac{2e}{h}\sum_q \bar{T}_{qp}\mu_p - \bar{T}_{pq}\mu_q \tag{2.41}$$

where $T_{qp} = T_{q\leftarrow p}$, and equivalently:

$$\begin{cases} I_p = \sum_q \left[G_{qp}V_p - G_{pq}V_q\right] \\ G_{pq} = \frac{2e^2}{h}\bar{T}_{pq} \end{cases} \tag{2.42}$$

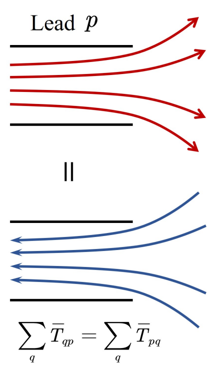
"Sum rule" for G_{pq}: current is zero when all V_p are equal:

$$0 = V\sum_q \left[G_{qp} - G_{pq}\right] \tag{2.43}$$

$$\Rightarrow \sum_q G_{qp} = \sum_q G_{pq} \quad \text{for } \forall p \tag{2.44}$$

$$\Rightarrow I_p = \sum_q G_{pq}[V_p - V_q] \tag{2.45}$$

$$= \sum_{q\neq p} G_{pq}[V_p - V_q] \tag{2.46}$$



Reciprocity: $[G_{qp}]_{+B} = [G_{pq}]_{-B}$ (To be proved).

Potential V_p at a voltage probe

$$I_p = 0 = \sum_q G_{pq}[V_p - V_q] \tag{2.47}$$

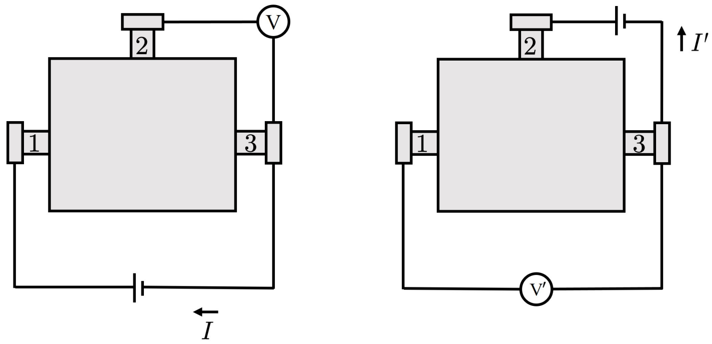
$$V_p = \frac{\sum_q G_{pq} V_q}{\sum_q G_{pq}} \tag{2.48}$$

Weighted average of all other terminal potentials. Weighting: G_{pq}.

Remark This formula gives us a way of understanding what a voltage probe measures when it is in contact with a system that does not have a well-defined local thermodynamic equilibrium.

The shape and construction of the probes affects the measured potential through the transmission functions. In a typical transports experiment, a current source is imposed, and the response voltages are measured. In the theory, we usually calculate the transmission and so the conductance tensor, and then obtain the resistance tensor by inversion $[R] = [G]^{-1}$.

2.4.2 Three-terminal device



Resistance: $R_{3t} = \frac{V}{I}$, $R'_{3t} = \frac{V'}{I'}$, According to the Büttiker formula, we obtain:

$$I_p = \sum_{q \neq p} G_{pq}[V_p - V_q] \tag{2.49}$$

$$\begin{cases} I_1 = (G_{12} + G_{13})V_1 - G_{12}V_2 - G_{13}V_3 \\ I_2 = (G_{21} + G_{23})V_2 - G_{21}V_1 - G_{23}V_3 \\ I_3 = (G_{31} + G_{32})V_3 - G_{31}V_1 - G_{32}V_2 \end{cases} \tag{2.50}$$

equally

$$\begin{pmatrix} I_1 \\ I_2 \\ I_3 \end{pmatrix} = \begin{pmatrix} G_{12} + G_{13} & -G_{12} & -G_{13} \\ -G_{21} & G_{21} + G_{23} & -G_{23} \\ -G_{31} & -G_{32} & G_{31} + G_{32} \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix} \tag{2.51}$$

Certain constraints are associated with these systems:

1. These equations are not independent, Kirchhoff's law $\sum_{i=1}^{3} I_i = 0$.
2. Only voltage differences matter, with a redundant voltage e.g. set $V_3 = 0$.

Then

$$\begin{pmatrix} I_1 \\ I_2 \end{pmatrix} = \begin{pmatrix} G_{12}+G_{13} & -G_{12} \\ -G_{21} & G_{21}+G_{23} \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \end{pmatrix} \quad \text{and} \quad I_3 = -I_1 - I_2 \tag{2.52}$$

$$\Rightarrow \begin{pmatrix} V_1 \\ V_2 \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \begin{pmatrix} I_1 \\ I_2 \end{pmatrix}, \qquad [R] = \begin{pmatrix} G_{12}+G_{13} & -G_{12} \\ -G_{21} & G_{21}+G_{23} \end{pmatrix}^{-1} \tag{2.53}$$

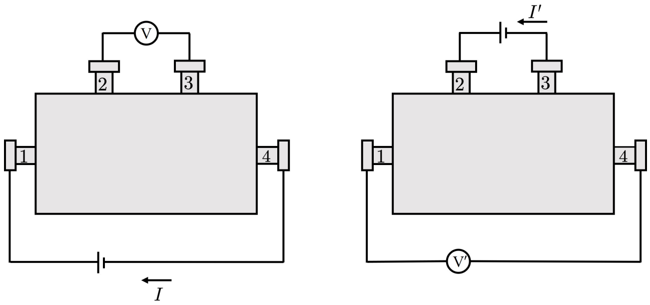
thus, the resistance can be determined:

$$R_{3t} = \frac{V}{I} = \left[\frac{V_2}{I_1}\right]_{I_2=0} = R_{21} \tag{2.54}$$

$$R'_{3t} = \frac{V'}{I'} = \left[\frac{V_1}{I_2}\right]_{I_1=0} = R_{12} \tag{2.55}$$

Remark We only focus on the magnitudes there, and don't care about the signs.

2.4.3 Four-terminal device



$$\begin{pmatrix} I_1 \\ I_2 \\ I_3 \\ I_4 \end{pmatrix} = \begin{pmatrix} G_{12}+G_{13}+G_{14} & -G_{12} & -G_{13} & -G_{14} \\ -G_{21} & G_{21}+G_{23}+G_{24} & -G_{23} & -G_{24} \\ -G_{31} & -G_{32} & G_{31}+G_{32}+G_{34} & -G_{34} \\ -G_{41} & -G_{42} & -G_{43} & G_{41}+G_{42}+G_{43} \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \end{pmatrix} \tag{2.56}$$

Set $V_4 = 0$, also we have $I_4 = -I_1 - I_2 - I_3$, We subsequently focus exclusively on this segment of the aforementioned equation:

$$\begin{pmatrix} I_1 \\ I_2 \\ I_3 \end{pmatrix} = \begin{pmatrix} G_{12}+G_{13}+G_{14} & -G_{12} & -G_{13} \\ -G_{21} & G_{21}+G_{23}+G_{24} & -G_{23} \\ -G_{31} & -G_{32} & G_{31}+G_{32}+G_{34} \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix} \tag{2.57}$$

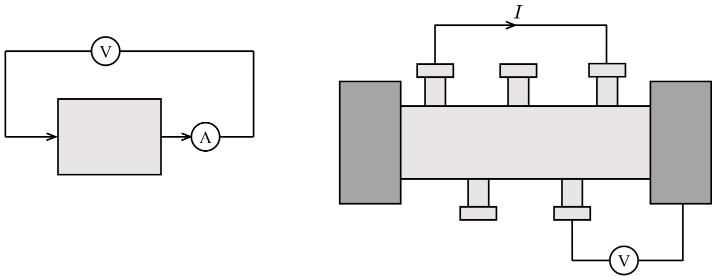
Inverting the conductance matrix yields the resistance matrix:

$$\begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22}+R_{23} & \\ R_{31} & R_{32} & R_{33} \end{pmatrix} \begin{pmatrix} I_1 \\ I_2 \\ I_3 \end{pmatrix}, \qquad [R] = [G]^{-1} \tag{2.58}$$

$$R_{4t} = \frac{V}{I} = \left[\frac{V_2 - V_3}{I_1}\right]_{I_2=I_3=0} = R_{21} - R_{31} \tag{2.59}$$

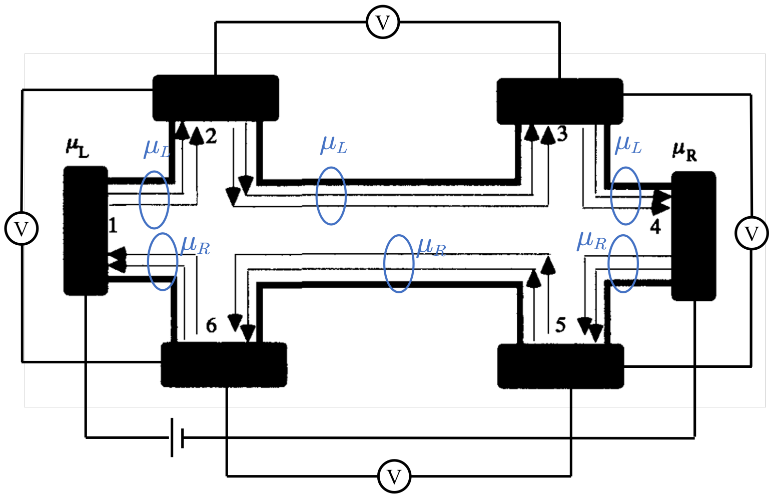
$$R'_{4t} = \frac{V'}{I'} = \left[\frac{V_1}{I_2}\right]_{I_1=I_4=0, I_2=-I_3} = R_{12} - R_{13} \tag{2.60}$$

2.4.4 Nonlocal Transport (two typical examples above)



Two implications: (i) Mesoscopic transport lacks of local picture, i.e. conducting loses its meaning (ii) Non-local measurement: Multiple probes and terminals. Both voltage probes and current probes should be specified to define the measurement.

Example 2.1 Quantum Hall effect (macroscopic scale, chiral edge states Hall bridge, filling factor $\nu = 2$, long



coherence length)

$$\begin{array}{ccccccc} G_{pq} & q=1 & 2 & 3 & 4 & 5 & 6 \\ p=1 & 0 & 0 & 0 & 0 & 0 & G_c \\ 2 & G_c & 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & G_c & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & G_c & 0 & 0 & 0 \\ 5 & 0 & 0 & 0 & G_c & 0 & 0 \\ 6 & 0 & 0 & 0 & 0 & G_c & 0 \end{array} \tag{2.61}$$

where $G_c = \frac{2e^2}{h} M$ ($M = 2$ when $\nu = 2$), and it should be multiplied by $\frac{1}{2}$ in the case of spin polarization. We only count direct connections! Contact 4 is assumed grounded $V_4 = 0$, and $I_p = \sum_q G_{pq}[V_p - V_q]$, so

$$\begin{pmatrix} I_1 \\ I_2 \\ I_3 \\ I_5 \\ I_6 \end{pmatrix} = \begin{pmatrix} G_c & 0 & 0 & 0 & -G_c \\ -G_c & G_c & 0 & 0 & 0 \\ 0 & -G_c & G_c & 0 & 0 \\ 0 & 0 & 0 & G_c & 0 \\ 0 & 0 & 0 & -G_c & G_c \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ V_5 \\ V_6 \end{pmatrix} \tag{2.62}$$

Remark Electron do not change the chemical potential during propagation: (i) Incident electrons possess the same distributions of the contacts. (ii) voltage probes have zero current, meaning the incident and outgoing electrons for the voltage probe have also the same distribution.

All voltage terminals have zero current:

$$I_2 = I_3 = I_5 = I_6 = 0 \tag{2.63}$$

thus we obtain:

$$V_1 = V_2 = V_3 \qquad V_5 = V_6 = 0 \tag{2.64}$$

$$I_1 = G_c V_1 \qquad I_4 = -I_1 \tag{2.65}$$

Longitudinal resistance R_L measured between 2 and 3, or between 5 and 6 is zero (Explains why DOS$=0$ is the bulk corresponds to minimal resistance):

$$R_L = \frac{V_2 - V_3}{I_1} = \frac{V_6 - V_5}{I_1} = 0 \qquad \text{(Dissipationless!)} \tag{2.66}$$

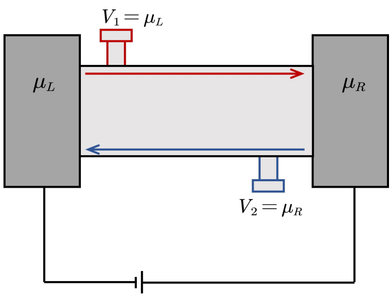
Hall resistance R_H measured between 2 and 6, or between 3 and 5 is quantized:

$$R_H = \frac{V_2 - V_6}{I_1} = \frac{V_3 - V_5}{I_1} = \frac{V_1}{I_1} = G_c^{-1} \qquad \text{(Quantized!)} \tag{2.67}$$

The longitudinal voltage drop V_L as measured by two voltage probes located anywhere on the same side of the sample is zero. The transverse (Hall) voltage V_H measured by two probes located anywhere on opposite sides of the sample is equal to the applied voltage:

$$V_L = 0, \qquad eV_H = \mu_L - \mu_R \tag{2.68}$$

This is the only when μ_L, μ_R lie in the gap between Landau levels. If μ_L, μ_R close to Landau levels, backscattering takes place through the bulk states, which gives rise to dissipasions and finite resistance.

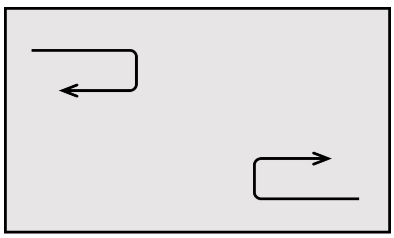


Edge state in equilibrium with μ_L and μ_R.

Note *A two-terminal resistance measurement would yield the Hall resistance. Only a four-terminal measurement with voltage probes located on the same side of the sample yields zero resistance.*

In this scenario, measuring Hall resistance is equivalent to a two terminal Longitudinal resistance measurement of Fig.1, the remarkable accuracy on the order of 10^{-10}.

Remark The net current is carried by the edge states does not mean that there is no spatial current distribution is the bulk.



Exercise 2.1 (E.4.1, page 194) Consider a slightly simplified form of the structure shown in Fig. 4.2.2, as shown in Fig. E.4.

(a) Write down the conductance matrix for this structure assuming that there is no communication between edge states as they propagate from the constriction to terminal 3.

(b) Use the Büttiker formula (Eq. (2.5.8)) to show that the Hall resistance is given by

$$R_H = \frac{V_2 - V_3}{I} = \frac{h}{2e^2 M}\frac{1}{1-p}$$

as reasoned in the text.

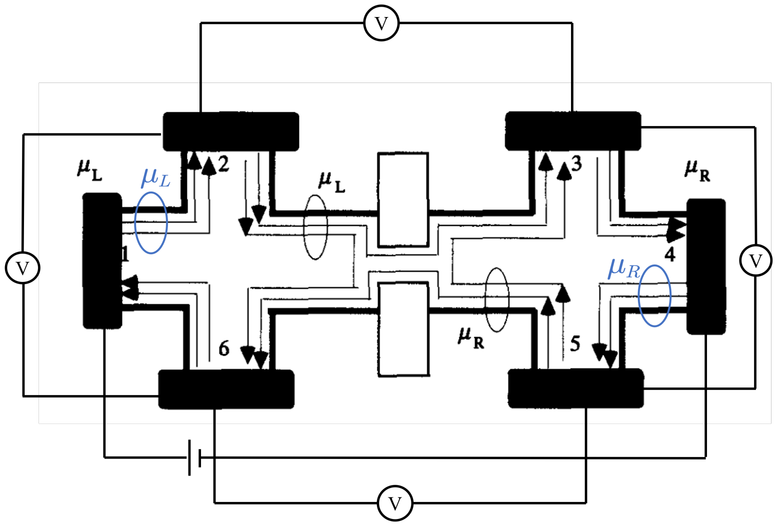
✍ **Exercise 2.2 (E.4.2, page 194)** Consider the same structure as in E.4.1 but with an extra terminal '5' inserted, as shown in Fig. E.4.2.

Write down the conductance matrix for this structure and show that the Hall resistance is now given by

$$R_H = \frac{V_2 - V_3}{I} = \frac{h}{2e^2 M}$$

The extra terminal establishes equilibrium between the edge states and changes the Hall resistance. This is a rather surprising result which has been ovserved experimentally. In macroscopic conductors, we do not expexted an extra floating probe ('5') to affect the measurement.

Example 2.2 QPC in Quantum Hall, effect of backscattering



The total number of channels is denoted by M, with $N(< M)$ channels facilitating complete transmission. Consequently, $M - N$ channels are characterized by complete backscattering.

$$I_1 = 2\frac{2e^2}{h}NV_1 \qquad (\mu_L = eV_1, \mu_R = eV_4 = 0) \tag{2.69}$$

$$I_1 = \frac{2e^2}{h}MV_1\frac{N}{M} = \frac{2e^2}{h}MV_1(1-p) \quad p = 1 - \frac{N}{M} \tag{2.70}$$

$$\mu_2 = \mu_L = eV_1, \qquad \mu_5 = 0 \quad \text{equilibrium with the incident contacts} \tag{2.71}$$

The contact 6 sees $M - N$ channels originating from the left and having a potential μ_L, and N channels originating from the right and having a potential μ_R. Using the formula for a floating terminal p:

$$V_p = \frac{\sum_{q\neq p} G_{pqV_q}}{\sum_{q\neq p} G_{pq}} \tag{2.72}$$

$$\Rightarrow \mu_6 = \frac{(M-N)\mu_L + N\mu_R}{M} = eV_1 p \tag{2.73}$$

Similarly for contact 3

$$\mu_3 = \frac{N\mu_L + (M-N)\mu_R}{M} = eV_1(1-p) \tag{2.74}$$

$$\Rightarrow R_L = \frac{V_2 - V_3}{I_1} \tag{2.75}$$

$$= \frac{V_1 - V_1(1-p)}{I_1} = \frac{V_1}{I_1}p = \frac{h}{2e^2M}\left[\frac{p}{1-p}\right] \tag{2.76}$$

$$= \frac{h}{2e^2M}\left[-1 + \frac{1}{1-p}\right] = \frac{h}{2e^2M}\left[\frac{M}{N} - 1\right] = \frac{h}{2e^2}\left[\frac{1}{N} - \frac{1}{M}\right] \tag{2.77}$$

Such fractional quantized longitudinal resistance has been observed.

At the same time, the Hall resistance R_H is unchanged:

$$R_H = \frac{V_2 - V_6}{I_1} = \frac{V_1(1-p)}{I_1} = \frac{h}{2e^2M} = \frac{V_3 - V_5}{I_1} \tag{2.78}$$

The above results can be obtained directly by the Büttiker formula.

$$\begin{array}{ccccccc} G_{pq} & q=1 & 2 & 3 & 4 & 5 & 6 \\ p=1 & 0 & 0 & 0 & 0 & 0 & G_c = \frac{2e^2}{h}M \\ 2 & G_c & 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & (1-p)G_c & 0 & 0 & pG_c & 0 \\ 4 & 0 & 0 & G_c & 0 & 0 & 0 \\ 5 & 0 & 0 & 0 & G_c & 0 & 0 \\ 6 & 0 & pG_c & 0 & 0 & (1-p)G_c & 0 \end{array} \tag{2.79}$$

We setting $V_4 = 0$, using $I_p = \sum_q G_{pq}[V_p - V_q]$:

$$\begin{pmatrix} I_1 \\ I_2 \\ I_3 \\ I_5 \\ I_6 \end{pmatrix} = \begin{pmatrix} G_c & 0 & 0 & 0 & -G_c \\ -G_c & G_c & 0 & 0 & 0 \\ 0 & -(1-p)G_c & G_c & -pG_c & 0 \\ 0 & 0 & 0 & G_c & 0 \\ 0 & -pG_c & 0 & -(1-p)G_c & G_c \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ V_5 \\ V_6 \end{pmatrix} \tag{2.80}$$

and

$$\begin{cases} I_2 = I_3 = I_5 = I_6 = 0 \\ V_2 = V_1, V_5 = 0 \end{cases} \Rightarrow \begin{cases} -(1-p)G_cV_2 + G_cV_3 = 0 \\ -pG_cV_2 + G_cV_6 = 0 \\ I_1 = G_c(V_1 - V_6) = G_c(1-p)V_1 \end{cases} \tag{2.81}$$

$$\tag{2.82}$$

so

$$V_3 = (1-p)V_2 = (1-p)V_1 \tag{2.83}$$

$$V_6 = pV_2 = pV_1 \tag{2.84}$$

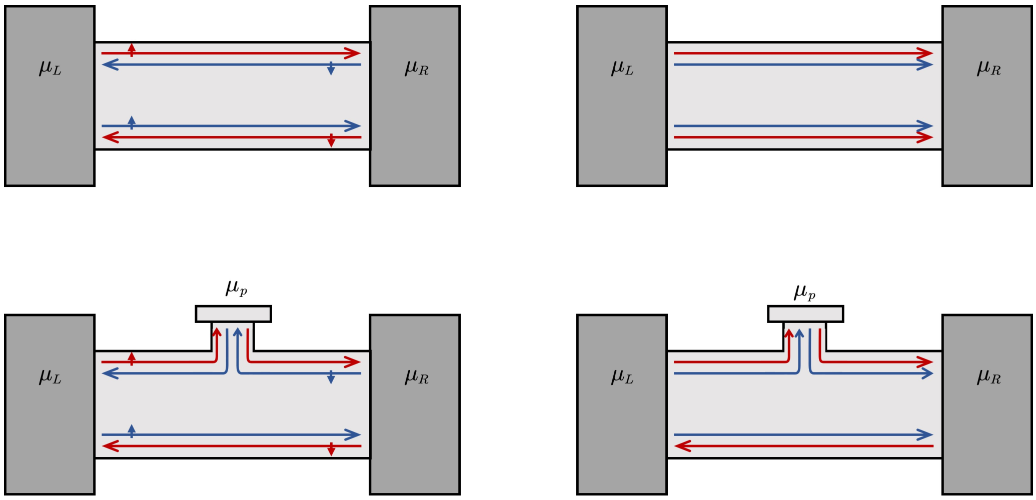
$$R_L = \frac{V_2 - V_3}{I_1} = \frac{V_6 - V_5}{I_1} = \frac{V_1}{I_1}p \tag{2.85}$$

$$R_H = \frac{V_2 - V_6}{I_1} = \frac{V_3 - V_5}{I_1} = \frac{V_1}{I_1}(1-p) \tag{2.86}$$

Example 2.3 Helical edge states in QSH (2D TI)

Conductance measure: No different between A & B, conductance $G = \frac{2e^2}{h}$.

Question: *How to distinguish Quantum Hall edge state and helical edge state?*



Answer: *Add a voltage probe!*

$$\begin{array}{cccc} G_{pq} & q=1 & 2 & 3 \\ p=1 & 0 & G_c & G_c = \frac{e^2}{h} \\ 2 & G_c & 0 & G_c \\ 3 & G_c & G_c & 0 \end{array} \tag{2.87}$$

considering $V_3 = 0$ and $I_3 = -I_1 - I_2$:

$$\begin{pmatrix} I_1 \\ I_2 \end{pmatrix} = \begin{pmatrix} 2G_c & -G_c \\ -G_c & 2G_c \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \end{pmatrix} \tag{2.88}$$

probe 2 is a voltage probe:

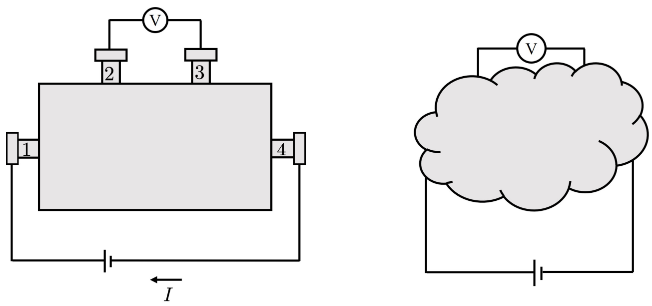
$$I_2 = 0 \Rightarrow V_1 = 2V_2 \Rightarrow V_2 = \frac{V_1}{2} \tag{2.89}$$

$$\Rightarrow I_1 = 2G_cV_1 - G_cV_2 = \frac{3}{2}G_cV_1 \tag{2.90}$$

$$\Rightarrow G = \frac{I_1}{V_1} = \frac{3}{2}G_c \tag{2.91}$$

Remark The Landauer-Büttiker formula is really successful in interpreting edge transport. In these cases, the scattering between different leads is really simple. In general quantum transport problems. However, the scattering itself is the main task to solve.

2.4.5 Reciprocity



Onsager relation $\begin{cases} \rho_{xx}(B) = \rho_{xx}(-B) & \text{(1) Symmetric} \\ \rho_{xy}(B) = -\rho_{yx}(-B) & \text{(2) Anti-symmetric} \end{cases}$

Question: *Does the symmetric equation of the Onsager relation imply that $R_{4t}(B) = R_{4t}(-B)$?*

Answer: *R_{4t} is neither symmetric nor antisymmetric. (i) Current flow on a mesoscopic scale is very irregular due to random scattering and not directed along x or y even in rectangular conductor. R_{4t} is some average of ρ_{xx} and ρ_{xy}. (ii) The same phenomenon is large conductors with irregular shapes.*

Reverse magnetic field, reverse the current and voltage probes, we will prove that for 3-terminal and 4-terminal, $R_{3t}(B) = R'_{3t}(-B)$ and $R_{4t}(B) = R'_{4t}(-B)$:

$$I_p = \sum_q G_{pq}[V_p - V_q] \iff I = \hat{G}V \iff \begin{pmatrix} I_1 \\ \vdots \\ I_N \end{pmatrix} = \begin{pmatrix} & & \\ & \hat{G} & \\ & & \end{pmatrix} \begin{pmatrix} V_1 \\ \vdots \\ V_N \end{pmatrix} \tag{2.92}$$

$$\hat{G} = [R]^{-1} = \begin{pmatrix} \ddots & & -G_{pq} \\ & \sum_{q \neq p} G_{pq} & \\ & & \ddots \end{pmatrix} \tag{2.93}$$

so $[\hat{G}]_{pp} = \sum_{q \neq p} G_{pq}$[1] is the diagonal element, and $[\hat{G}]_{pq} = -G_{pq}$ is the off-diagonal element. We demonstrate this relationship through a two-step process, focusing first on the off-diagonal elements and then on the diagonal elements:

(1) Off-diagonal elements: $[R^{-1}]_{pq} = -G_{pq}$.

This can be directly demonstrated using the reciprocity of the conductance coefficient:

$$[G_{qp}]_B = [G_{pq}]_{-B} \tag{2.94}$$

$$\Rightarrow [R^{-1}]^B_{pq} = [R^{-1}]^{-B}_{qp} \tag{2.95}$$

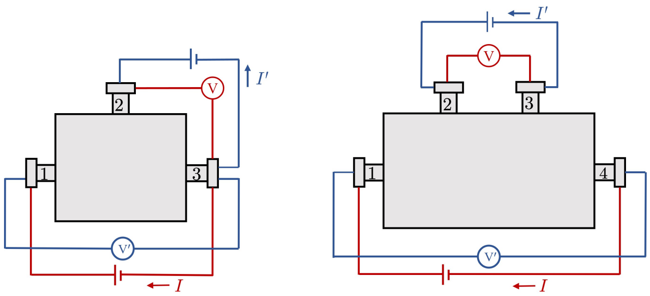
(2) Diagonal elements

$$\begin{cases} \sum_q [G_{pq}]_B = \sum_q [G_{qp}]_B = \sum_q [G_{pq}]_{-B} \\ [G_{pp}]_B = [G_{pp}]_{-B} \end{cases} \Rightarrow [R^{-1}]^B_{pp} = \sum_{q \neq p} [G_{pq}]_B = \sum_{q \neq p} [G_{pq}]_{-B} = [R^{-1}]^{-B}_{pp} \tag{2.96}$$

Using Eq. (2.95) and (2.96), we deduce that:

$$[R^{-1}]_B = [R^{-1}]^T_{-B} = [R^T]^{-1}_{-B} \tag{2.97}$$

$$\Rightarrow [R]_B = [R^T]_{-B} \tag{2.98}$$



[1] G_{pq} represents the conductance coefficients, indicating scattering probability, whereas $\hat{G}$ refers to the conductance matrix.

- 3-Terminal case: $R_{3t}(B) = R_{21}(B) = R'_{3t}(-B) = R_{12}(-B)$
- 4-Terminal case: $R_{4t}(B) = R_{21}(B) - R_{31}(B) = R'_{4t}(-B) = R_{12}(-B) - R_{13}(-B)$

Remark The correct prediction of the reciprocity properties observed experimentally in 4-Terminal mesoscopic structures was the first important application of the Büttiker formula. Many interesting phenomena are all related to the non-intuitive behavior of mesoscopic voltage probes. They require us to view the probes as extensions of the waveguide itself and calculate the resistance of the composite probe-device configuration.

✍ **Exercise 2.3 (E.2.3, page 113)** Consider a cross junction as shown in Fig. E.1. Assuming that the four ports are completely symmetric, we can define a coefficient for forward transmission, one for right turning and for left turning as follows:

$$\bar{T}_{13} = \bar{T}_{31} = \bar{T}_{42} = \bar{T}_{24} = T_F$$
$$\bar{T}_{21} = \bar{T}_{31} = \bar{T}_{43} = \bar{T}_{14} = T_R$$
$$\bar{T}_{41} = \bar{T}_{12} = \bar{T}_{23} = \bar{T}_{34} = T_L$$

We have reproduced the measured values of T_F, T_L and T_R as a function of the magnetic field from *Phys. Rev. B*, **46**, 9653-4 (1992). See this reference for a description of how the transmission functions are measured.

(a) Suppose we measure the Hall resistance R_H by running a current from 1 to 3 and measuring the voltage between 2 and 4. Show that

$$R_H = \frac{h}{2e^2}\frac{T_R^2 - T_L^2}{(T_R + T_L)[T_R^2 + T_L^2 + 2T_F(T_F + T_R + T_L)]}$$

(b) Use the data provided above to calculate R_H vs. B numerically from the relation derived in part (a).

✍ **Exercise 2.4 (E.2.4, page 114)** We would expect the conductance of two apertures in series to be half that of a single aperture: $G = M(2e^2/h) \times 0.5$. But if the two apertures are sufficiently close together then the electrons emerging from one aperture do not have the chance to spread out before they reach the second aperture. Consequently the conductance is the same as that of a single aperture: $G = M(2e^2/h)$. But if we turn on a magnetic field then the electrons get deflected and the conductance is reduced (see A. A. M. Staring *et al*. (1990), *Phys. Rev. B*, **41**, 8461). Use the Büttiker formula to show that the conductance is given by (see C. W. J. Beenakker and H. van Houten (1989), *Phys. Rev. B*, **39**, 10445)

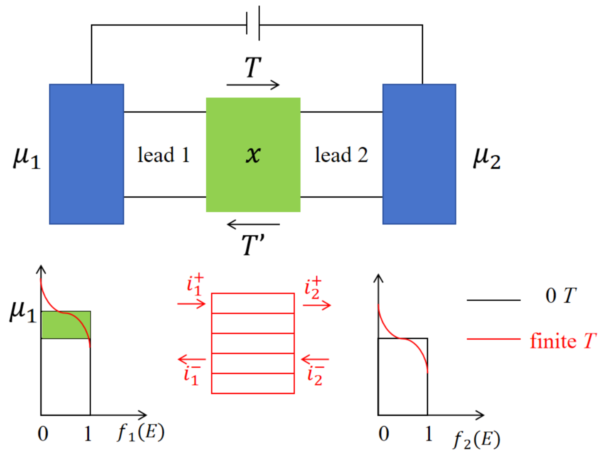
$$G = (e^2/h)\left[M + T_F + \frac{(T_R - T_L)^2}{2T'_F + T_R + T_L}\right]$$

where

$$\bar{T}_{13} = \bar{T}_{31} = T_F$$
$$\bar{T}_{42} = \bar{T}_{24} = T'_F$$
$$\bar{T}_{21} = \bar{T}_{32} = \bar{T}_{43} = \bar{T}_{14} = T_R$$
$$\bar{T}_{41} = \bar{T}_{12} = \bar{T}_{23} = \bar{T}_{34} = T_L$$

2.5 Non-zero temperature and bias

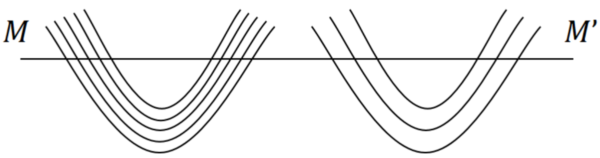
Previously, for the derivation of Landauer formula we assume: (1) zero temperature, (2) Energy-independent transmission probability. In general, we concentrate on the energy range: μ_1+(a few k_BT)> $E > \mu_2$−(a few k_BT). Injection from both contacts:



Influx per unit energy from lead 1: $i_1^+(E) = (2e/h)Mf_1(E)$, where M is the number of transverse modes, f_1 is the Fermi distribution of lead 1. Influx per unit energy from lead 2: $i_2^-(E) = (2e/h)M'f_2(E)$, where M may denote different transverse modes, f_2 is another Fermi distribution. Outflux from lead 2: $i_2^+(E) = Ti_1^+(E) + (1-T')i_2^-(E)$, where T is the average transmission probability. Outflux from lead 1: $i_1^-(E) = (1-T)i_1^+(E) + T'i_2^-(E)$. The net current $i(E)$ flowing at any point (left or right lead):

$$\begin{aligned} i(E) &= i_1^+ - i_1^- = i_2^+ - i_2^- = Ti_1^+(E) - T'i_2^-(E) \\ &= \frac{2e}{h}[M(E)T(E)f_1(E) - M'(E)T'(E)f_2(E)] = \frac{2e}{h}[\overline{T}(E)f_1(E) - \overline{T'}(E)f_2(E)] \end{aligned} \tag{2.99}$$

where $\overline{T}(E) = M(E)T(E) = \sum_{n=1}^{M} T_n(E)$.



Total current:

$$I = \int i(E)dE = \frac{2e}{h}\int [\overline{T}(E)f_1(E) - \overline{T'}(E)f_2(E)]dE \tag{2.100}$$

If $\overline{T}(E) = \overline{T'}(E) \Rightarrow$

$$I = \frac{2e}{h}\int \overline{T}(E)[f_1(E) - f_2(E)]dE \tag{2.101}$$

[Note: (1) $i(E) = 0$ when $f_1 = f_2 \Rightarrow \overline{T}(E) = \overline{T'}(E)$. This holds only at equilibrium. (2) No inelastic scattering, $\overline{T}(E) = \overline{T'}(E)$ always holds for two-terminal device even with magnetic field.]

How about quantum hall and quantum spin hall?

2.5.1 linear response

$I \propto V$, the current is proportional to small bias voltage. Small deviation from equilibrium by voltage bias: $\delta\mu = \mu_1 - \mu_2$. Starting with equilibrium $\mu_1 = \mu_2$ and then apply a bias, $\mu_1 = \mu_2 + \delta\mu$,

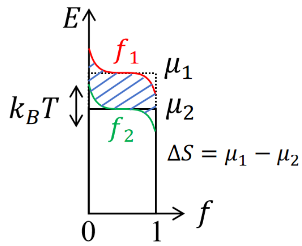
$$\delta I = \frac{2e}{h}\delta\int \overline{T}(E)[f_1(E) - f_2(E)]dE = \frac{2e}{h}\int \{[\overline{T}(E)]_{eq}\delta[f_1 - f_2] + [f_1 - f_2]_{eq}\delta[\overline{T}(E)]\}dE \tag{2.102}$$

The equilibrium condition is $[f_1 - f_2]_{eq} = 0$, and $\delta[f_1 - f_2] \simeq \left[\frac{\partial f_2}{\partial \mu_2}\right]_{eq} \delta\mu = \left(-\frac{\partial f_2}{\partial E}\right)\delta\mu$, where we have used $\partial_\mu = -\partial_E$. $f_0 = f_2(E) = \frac{1}{\exp[(E-\mu_2)/k_BT]+1}\Big|_{\mu_2=\mu}$. Linear response: differential conductance equals the conductance. $G = e\frac{\delta I}{\delta\mu} = \frac{2e^2}{h}\int \overline{T}(E)\left[-\frac{\partial f_0(E)}{\partial E}\right]dE$. For low temperature, $f_0(E) \simeq \theta(E_F - E) \Rightarrow -\frac{\partial f_0(E)}{\partial E} \simeq \delta(E_F - E) \Rightarrow G = \frac{2e^2}{h}\overline{T}(E_F)$

2.5.2 When is the response linear?

Condition for Taylor expansion: $\delta\mu \ll k_BT$, since the typical energy scale at which f_0 varies is $\sim k_BT$. (Sufficient condition, not necessary condition. Otherwise, no linear response at zero temperature.)

Relaxed condition for temperature-independent linear response: $\overline{T}(E)$ $\simeq$constant over the energy range of transport, and unaffected by the bias. For low temperature, or relatively high temperatures, as long as $k_BT \ll \mu_1, \mu_2$, we have $I = \frac{2e}{h}\overline{T}(E_F)\delta\mu$.



2.5.3 General criterion for linear response

$$I = \frac{2e}{h}\int \overline{T}(E)[f_1 - f_2]dE = \frac{2e}{h}\int_{-\infty}^{\infty}\overline{T}(E)\left[\frac{1}{e^{(E-\mu_1)/k_BT}+1} - \frac{1}{e^{(E-\mu_2)/k_BT}+1}\right]dE \tag{2.103}$$

$$f_1(E) - f_2(E) = \int_{\mu_1}^{\mu_2}\frac{d}{dE'}\frac{1}{e^{(E-E')/k_BT}+1}dE' = \int_{\mu_1}^{\mu_2} -\frac{d}{d(E-E')}\frac{1}{e^{(E-E')/k_BT}+1}dE' \tag{2.104}$$

Define

$$F_T(E) = -\frac{d}{dE}\left(\frac{1}{e^{E/k_BT}+1}\right) = \frac{1}{4k_BT}\mathrm{sech}^2(\frac{E}{k_BT}) \tag{2.105}$$

where we have used $(\frac{1}{e^x+1})' = \frac{1}{(e^{x/2}+e^{-x/2})^2} = \frac{1}{4}\mathrm{sech}^2 x$. Thus

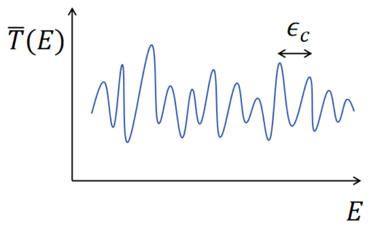
$$\begin{aligned} f_1(E) - f_2(E) &= \int_{\mu_1}^{\mu_2} F_T(E-E')dE' \\ \Rightarrow I &= \frac{2e}{h}\int \overline{T}(E)dE\int_{\mu_1}^{\mu_2} F_T(E-E')dE' \\ = \frac{1}{e}\int_{\mu_1}^{\mu_2}&\left[\frac{2e^2}{h}\int\overline{T}(E)F_T(E-E')dE\right]dE' = \frac{1}{e}\int_{\mu_1}^{\mu_2}\widetilde{G}(E')dE' \end{aligned} \tag{2.106}$$

where we define $\frac{2e^2}{h}\int\overline{T}(E)F_T(E-E')dE$ as $\widetilde{G}(E')$. Linear response occurs when $\widetilde{G}(E')$ is independent of $E' \in [\mu_1, \mu_2]$, then $I = \widetilde{G}(E_F)\frac{\mu_1-\mu_2}{e}$,

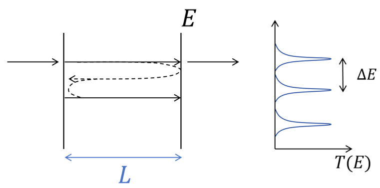
$$\begin{aligned} G = \widetilde{G}(E_F) &= \frac{2e^2}{h}\int\overline{T}(E)F_T(E-E_F)dE \\ = \frac{2e^2}{h}\int\overline{T}(E)&\left[-\frac{d}{dE}\frac{1}{e^{(E-E_F)/k_BT}+1}\right]dE = \frac{2e^2}{h}\int\overline{T}(E)[-\frac{\partial f_0}{\partial E}]dE \end{aligned} \tag{2.107}$$

which is in agreement with obtained by linear expansion.

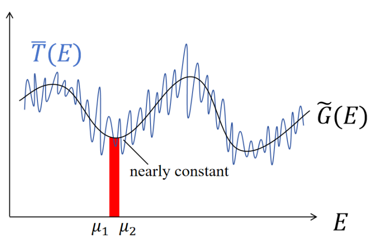
Physical regime (1): sharp resonant structures of $\overline{T}(E)$. Low temperature, long $\tau_\phi \Rightarrow$ strong quantum interference. For a diffusive conductor, the correlation energy $\varepsilon_c \simeq \frac{\hbar}{\tau_\phi}$. For $\tau_\phi = 100$ps, $\varepsilon_c \to 0.006$meV.



This can be understood as follows. Consider double barrier resonance with perfect coherence: $\tau_\phi = \infty$. $2k \cdot L = 2n\pi$, $n = 1, 2, ...$, $\Delta k = \frac{\pi}{L}$, $\Delta\varepsilon = \frac{\partial\varepsilon}{\partial k}\Delta k = \hbar v_F \Delta k = \hbar v_F \cdot \frac{\pi}{L} \sim \frac{\hbar}{\tau}$, $\tau = \frac{L}{v_F}$ is the time spent within the barrier.



For diffusive conductors, there are many long interference trajectories. Many of them are longer than coherence length, or $L_t > L_\phi \Leftrightarrow \tau > \tau_\phi$. For these trajectories, decoherence takes place, reduces to classical behavior. For those trajectories with $L_t < L_\phi \Leftrightarrow \tau < \tau_\phi$, strong interference occurs, then for them, the picture is similar to the double barrier resonance, with L replaced by $L_t \sim L_\phi \Rightarrow \tau = \tau_\phi = \frac{L_\phi}{v_F} \Rightarrow \varepsilon_c \simeq \frac{\hbar}{\tau_\phi}$. Now re-examine: $\widetilde{G}(E') = \frac{2e^2}{h}\int \overline{T}(E)F_T(E-E')dE$. F_T smears out sharp structures in scale of $k_B T (\gg \varepsilon_c)$.



keeping only the fluctuations in larger scales, $k_B T$ is the relevant energy scale. $T = 0.1$k, $k_B T \simeq 0.01$meV. In this case, linear response condition changes into: $\mu \ll k_B T$. (For true zero-temperature, such smearing does not exist, then we need $\mu \ll \varepsilon_c$ to achieve linear response. Not the usual case.) In mesoscopic experiments the bias is always kept smaller than $k_B T$ to ensure linear response.

Physical regime (2): smooth $\overline{T}(E)$ with large correlation energy ε_c. $f_T(E)$ has small effect, and the relevant energy is ε_c. Condition for linear response: $\Delta\mu \ll \varepsilon_c$.

Combining (1) and (2) $\Rightarrow$ general criterion for linear response: $\Delta\mu \ll k_B T + \varepsilon_c$.

Remark For high bias, $\overline{T}(E) = \overline{T}(E, \mu_1, \mu_2)$. For small bias, $\overline{T}(E) \to \overline{T}(E, \mu_1 \simeq \mu_2 \simeq E_F)$

2.5.4 Multi-terminal conductors

Current is in any terminal (labeled by p) is contributed by both the incident and outgoing electrons. $I_p = \int i_p(E)dE$,

$$i_p(E) = \frac{2e}{h}\sum_q [\overline{T}_{qp}(E)f_p(E) - \overline{T}_{pq}(E)f_q(E)] = \frac{2e}{h}\sum_{q\neq p}[\overline{T}_{qp}(E)f_p(E) - \overline{T}_{pq}(E)f_q(E)] \tag{2.108}$$

$\overline{T}_{pq}(E)$: total transmission from terminal q to p at E, $f_p(E)$ is the Fermi-Dirac function in p. No current at equilibrium $\Rightarrow i_p = 0$

$$\Rightarrow \sum_q \overline{T}_{qp}(E) = \sum_q \overline{T}_{pq}(E) \Rightarrow i_p(E) = \frac{2e}{h}\sum_q \overline{T}_{pq}(E)[f_p(E) - f_q(E)] \tag{2.109}$$

Remark Far away from equilibrium, this relation is true only if no inelastic scattering exists.

Linear expansion:

$$\widetilde{G}_{pq}(E') = \frac{2e^2}{h}\int \overline{T}_{pq}(E)[f_p(E) - f_q(E)]dE \simeq \frac{e^2}{h}\int \overline{T}_{pq}(E)F_T(E-E_F)dE$$
$$= \int \overline{T}_{pq}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE = \widetilde{G}_{pq}(E_F) = G_{pq} \Rightarrow I_p = \frac{1}{e}\sum_q \int_{\mu_q}^{\mu_p} \widetilde{G}_{pq}(E')dE' \simeq \sum_q G_{pq}[V_p - V_q] \tag{2.110}$$

which is the Büttiker formula.

Question: *What is E_F? $E_F = \mu_p ? \frac{1}{2}(\mu_1 + \mu_2)$?*

Answer: *Not important in the linear response regime since $\widetilde{G}_{pq}(E')$ is independent of E' for $E' \sim \{u_p\}$. Only the chemical potential difference $\Delta\mu = \mu_p - \mu_q$ matters. For low temperatures and large correlation energy $\varepsilon_c \gg \mu_p - \mu_q$, $\widetilde{G}_{pq} \simeq \frac{2e^2}{h}\overline{T}_{pq}(E_F)$. Floating voltage probe: $I_p = 0$ rather than $i_p = 0$, $I_p = \int i_p(E)dE = 0$ to solve μ_p.*

Remark For multi-terminal conductors, this kind of method is really hard to apply. Any voltage probe one should use $I_p = 0$ as a constraint, in an indirect way. All the work on multi-terminal conductors is based on the linear response formula (Buttiker Formula). The V_p is an explicit parameter, which is not solved in a consistent way.

2.6 Exclusion principle?

Whether we should modify the current expression

$$i_p(E) = \frac{2e}{h}\sum_q \left[\bar{T}_{qp}f_p(E) - \bar{T}_{pq}f_q(E)\right] \tag{2.111}$$

to account for the exclusion principle[2]:

$$i_p(E) = \frac{2e}{h}\sum_q \left[\bar{T}_{qp}f_p(E)(1-f_q) - \bar{T}_{pq}f_q(E)(1-f_p)\right] \qquad \text{(Wrong!)} \tag{2.112}$$

The difference of above two equation:

$$\frac{2e}{h}\sum_q -\left[\bar{T}_{qp} - \bar{T}_{pq}\right] f_p f_q \tag{2.113}$$

It is zero if $\bar{T}_{qp} = \bar{T}_{pq}$. From the example of QH edge states, we have learnt that $\bar{T}_{qp} \neq \bar{T}_{pq}$, this is the general case.

[2]This is what we do in the Fermi's golden rule.

Note *Two-terminal without inelastic scattering, $\bar{T}_{qp} = \bar{T}_{pq}$. The distinction is not appreciated before Büttiker's work on multi-terminal devices.*

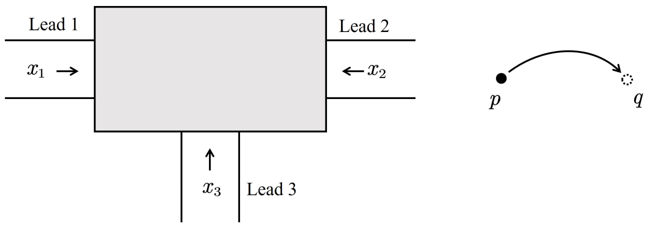
Question: *In the linear response regime, the Büttiker formula is the natural solution. Then why we care about whether Eq (2.111) or Eq (2.112) is correct?*

Answer: *G_{pq} is obtained by linearizing Eq (2.111) if we use Eq (2.112). the valve of G_{pq} is different.*

If transport is coherent across the conductor, so that we can define a single wavefunction extending from one lead to another, then Eq (2.111) is the correct expression for the current. Otherwise, the transport is not coherent, and then neither Eq (2.111) nor Eq (2.112) is correct.

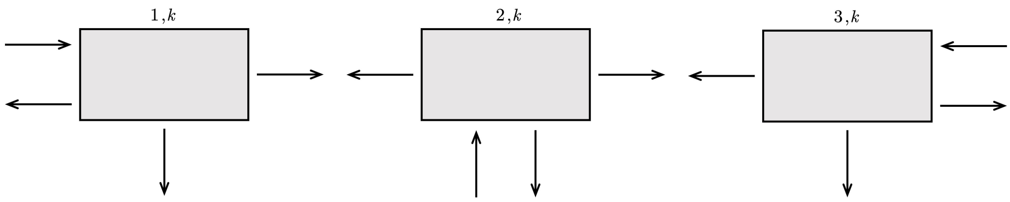
2.6.1 Scattering states

The concern of exclusion principle: transitions between localized eigenstate in different leads



$$|p,k\rangle \equiv \sin(kx_p) \overset{f_p(1-f_q)}{\longrightarrow} |q,k'\rangle \equiv \sin(k'x_q) \qquad \text{Standing waves} \tag{2.114}$$

The view is accurate when leads are *weakly coupled* to the conductor. In contrast, with *stronger couplings*, the lead eigenstates transform into scattering states. We should view the scattering states as whole, which are nonlocal and carry current. We are now talking about the occupation of these scattering states.



Wave function in lead p due to scattering state (q,k)

$$\psi_p(q) = \delta_{pq}\chi_p^+(y_p)e^{ik^+x_p} + S'_{pq}\chi_p^-(y_p)e^{ik^-x_p} \tag{2.115}$$

The first term represents the incident component, whereas the second term corresponds to the outgoing component, where S'_{pq} denotes the scattering amplitude.

A scattering state (q,k), if occupied, give rise to a current $i_p(q)$ per unit energy in lead p.

$$i_p(q) = \frac{2e}{h}(\delta_{pq} - T_{pq}) \qquad (\text{Note } T_{pq}, \text{ not } \bar{T}_{pq}) \tag{2.116}$$

Extending from a single transverse mode to multiple modes is a straightforward process.

The occupation of the scattering state (q,k) is determined by the occupation of the incident channel.

Total current: $I_p = \int \sum_q f_q(E) i_p(q) dE$

Remark Using equilibrium statistical mechanics to treat a non-equilibrium problem. Each eigenstate remains in equilibrium, but with a different reservoir, whose rule is the incident obeying the statistics of the relevant reservoir.

Picture of scattering state

$$I_p = \frac{2e}{h}\int \sum_q f_q(E)(\delta_{pq} - T_{pq})dE = \frac{2e}{h}\int [f_q - \sum_q T_{pq} f_q]dE \tag{2.117}$$

$$= \frac{2e}{h}\int [f_q(1 - T_{pp}) - \sum_{q\neq p} T_{pq} f_q]dE \tag{2.118}$$

where $1 - T_{pp}$ indicates that transmission from $p \to q \neq p$ is the incident minus reflected. Using sum rule:

$$\sum_q T_{pq} = \sum_q T_{qp} = 1 \qquad \text{(current conservation, prove later, similar to } \sum_q G_{pq} = \sum_q G_{qp}) \tag{2.119}$$

we derived that

$$I_p = \frac{2e}{h}\int [\sum_q T_{pq}(f_p - f_q)]dE = \frac{2e}{h}\int [\sum_{q\neq p} T_{qp} f_p - T_{pq} f_q]dE \tag{2.120}$$

The summation over $q \neq p$ signifies that only contain transmission between different leads.

Multiple modes in each lead, replace $T_{pq} \to \bar{T}_{pq}$:

$$\bar{T}_{pq} = \sum_{m\in p}\sum_{n\in q} T_{mn} \tag{2.121}$$

For the scattering, each mode (m, n) can be thought of as independent terminals. For the occupation, $m \in p$, $n \in q$ is different leads are different. This is the reason why we should specify which mode belonging to which lead, to define its distribution.

Question: *Whether the scattering states are orthogonal and complete?*

Answer: *Yes! To be proved later by scattering matrix theory.*

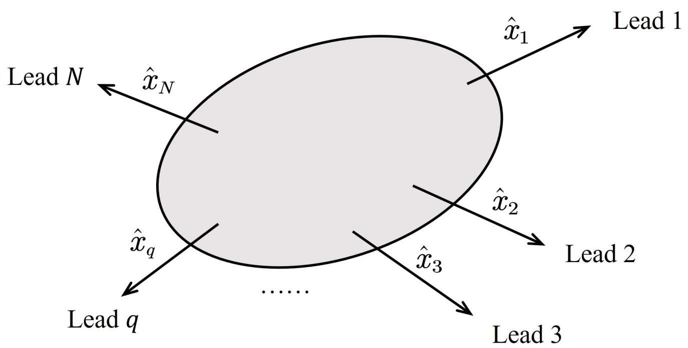
2.6.2 Scattering states with non-zero magnetic field

Question: *Magnetic field destroys translational symmetry of the leads. How can we express the scattering states as plane waves again?*

Answer: *Using Landau gauge $\vec{A} = -\hat{x}By$, $\hat{x}$ is the direction along the lead.*

Question: *How should we handle the case where different leads have their own $\hat{x}$ directions??*

Answer: *Choose gauge $\tilde{A} \sim \hat{x}_q B y_q$ in every lead q.*



It must impose restrictions on the gauge in the scattering region.

2.6.3 Different transverse modes, independent contribution to current

The transverse modes $\chi_p^{\pm}$ for the incident/scattering states may be different, e.g. in the presence of magnetic field, or SOC, etc. We begin with the definition of current:

$$\vec{J} = e[\psi(\hat{v}\psi)^* + \psi^*(\hat{v}\psi)] = \frac{e}{2m}[\psi(\hat{\Pi})^* + \psi^*(\hat{\Pi}\psi)] = \text{Re}[\frac{e}{m}\psi^*\hat{\Pi}\psi] \tag{2.122}$$

where $\hat{\Pi} = \hat{p} - e\vec{A}$ is the kinetic momentum, and $\hat{p} = -i\hbar\nabla$ is the canonical momentum.

The current flows in the $\hat{x}$ direction:

$$I = \int J_x(y)dy = \frac{e}{2m}\int \{\psi(r)[(p_x - eA_x)\psi(r)]^* + \psi^*(r)[(p_x - eA_x)\psi(r)]\}\, dy \tag{2.123}$$

The incident wave: $\psi_i = \frac{1}{\sqrt{L}}\chi^+(y)e^{ik^+x}$, where the $\chi^+(y)$ assume to be real. Thus, the current can be expressed as[3]:

$$I_i = \frac{e}{mL}\int [\chi^+(y)(\hbar k^+ - eA_x)\chi^+(y)]\, dy. \tag{2.124}$$

Scattered (outgoing) wave $\psi_s = s'\frac{1}{\sqrt{L}}\chi^-(y)e^{-ik^-x}$, from which the current is expressed as:

$$I_s = |s'|^2\frac{e}{mL}\int [\chi^-(\hbar k^- - eA_x)\chi^-]\, dy \tag{2.125}$$

The current should not be calculated separately, since the wavefunction is a superposition of both.

$$\psi = \chi_{k^+}^+(y)e^{ik^+x} + s'\chi_{k^-}^-(y)e^{ik^-x} \tag{2.126}$$

There are additional cross terms like

$$I_{cross} = \frac{e}{2m}\frac{1}{L}\left\{\int \chi_{k^+}^+(y)e^{ik^+x}\left[(\hbar k^- - eA_x)s'\chi_{k^-}^-(y)e^{ik^-x}\right]^* dy \right. \tag{2.127}$$

$$+\int s'\chi_{k^-}^-(y)e^{ik^-x}\left[(\hbar k^+ - eA_x)\right]^*\chi_{k^+}^+(y)e^{ik^+x}dy \tag{2.128}$$

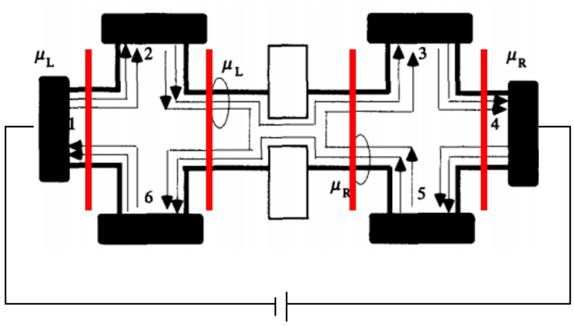
$$+\int \chi_{k^+}^+(y)e^{-ik^+x}\left[(\hbar k^- - eA_x)s'\chi_{k^-}^-(y)e^{ik^-x}\right] dy \tag{2.129}$$

$$\left. +\int s'\chi_{k^-}^-(y)e^{-ik^-x}\left[(\hbar k^+ - eA_x)\right]^*\chi_{k^+}^+(y)e^{ik^+x}dy \right\} \tag{2.130}$$

$$= \frac{e}{2m}\frac{1}{L}\left[s'e^{i(k^- - k^+)x}\int \chi^+[\hbar(k^+ + k^-) - 2eA_x]\chi^- dy + s'e^{i(k^+ - k^-)x}\int \chi^+[\hbar(k^+ + k^-) - 2eA_x]\chi^- dy\right] \tag{2.131}$$

Therefore, $I = I_i - I_s$, with I_i, I_s calculated separated by ψ_i, ψ_s.

Exercise 2.5 Calculate the current of the four sections as shown in Fig. E.1.



[3] have not sum over k

Solution

$$
\begin{array}{ccccccc}
G_{pq} & q=1 & 2 & 3 & 4 & 5 & 6 \\
p=1 & 0 & 0 & 0 & 0 & 0 & G_c = \frac{2e^2}{h}M \\
2 & G_c & 0 & 0 & 0 & 0 & 0 \\
3 & 0 & (1-p)G_c & 0 & 0 & pG_c & 0 \\
4 & 0 & 0 & G_c & 0 & 0 & 0 \\
5 & 0 & 0 & 0 & G_c & 0 & 0 \\
6 & 0 & pG_c & 0 & 0 & (1-p)G_c & 0
\end{array}
\tag{2.132}
$$

We set $V_4 = 0$*, using* $I_p = \sum_q G_{pq}[V_p - V_q]$*:*

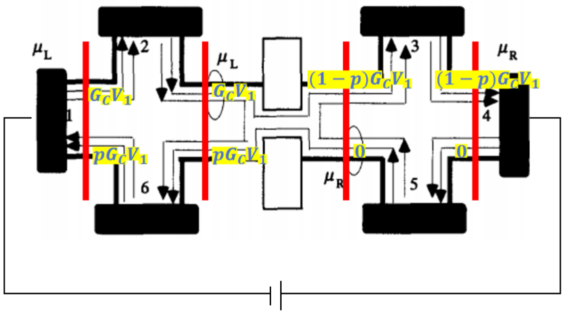
$$
\begin{pmatrix} I_1 \\ I_2 \\ I_3 \\ I_5 \\ I_6 \end{pmatrix} = \begin{pmatrix} G_c & 0 & 0 & 0 & -G_c \\ -G_c & G_c & 0 & 0 & 0 \\ 0 & -(1-p)G_c & G_c & -pG_c & 0 \\ 0 & 0 & 0 & G_c & 0 \\ 0 & -pG_c & 0 & -(1-p)G_c & G_c \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ V_5 \\ V_6 \end{pmatrix} \tag{2.133}
$$

and

$$
\begin{cases} I_2 = I_3 = I_5 = I_6 = 0 \\ V_2 = V_1, V_5 = 0 \end{cases} \Rightarrow \begin{cases} -(1-p)G_cV_2 + G_cV_3 = 0 \\ -pG_cV_2 + G_cV_6 = 0 \\ I_1 = G_c(V_1 - V_6) = G_c(1-p)V_1 \end{cases} \tag{2.134}
$$

$$
\tag{2.135}
$$

This can also be argued as follows:



Exercise 2.6 (E.2.6, page 115) Show that the following orthogonality relation

$$
\int \left[\chi_{m,k} \left(\frac{\hbar(k+k')}{2} + eBy \right) \chi_{n,k'} \right] dy = \delta_{k,k'}
$$

where the two functions $\chi_{m,k}(y)$ and $\chi_{n,k'}(y)$ satisfy

$$
\left[E_s + \frac{(\hbar k + eBy)^2}{2m} + \frac{p_y^2}{2m} + U(y) \right] \chi_{m,k}(y) = E\chi_{m,k}(y)
$$

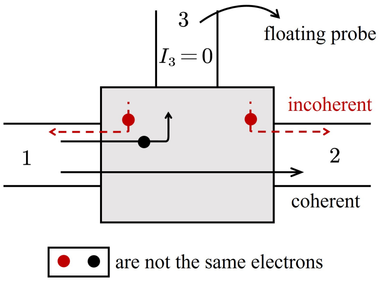
$$
\left[E_s + \frac{(\hbar k + eBy)^2}{2m} + \frac{p_y^2}{2m} + U(y) \right] \chi_{n,k'}(y) = E\chi_{n,k'}(y)
$$

which are appropriately normalized.

2.6.4 Non-coherent transport

Phenomenological approach: virtual voltage probe as a phase-breaking scatterer.

Scattering between lead 1-3 is coherent. Net current flows between lead 1 & 2, because $I_3 = 0$. Focusing on conductor and lead 1, 2, the system is an effectively open system, leading to decoherence. Physically, the electron transmitted into lead 3 and the electron the escape are not the same electron, thereby having no phase coherence. The virtual voltage can be used to simulate the decoherence effect.



$$i_p(E) = \frac{2e}{h}\sum_q \bar{T}_{pq}(E)[f_p(E) - f_q(E)] + \frac{2e}{h}\bar{T}_{p\varphi}(E)[f_p(E) - f_\varphi(E)] \tag{2.136}$$

The first term represents the real terminals, while the second term corresponds to the virtual probe. For the fictitious probe

$$i_\varphi(E) = \frac{2e}{h}\sum_q \bar{T}_{\varphi q}(E)[f_\varphi(E) - f_q(E)] \tag{2.137}$$

$$\Rightarrow f_\varphi(E) = \left(\frac{h}{2e}i_\varphi + \sum_q \bar{T}_{\varphi q}(E)f_q(E)\right)/\bar{R}_\varphi \tag{2.138}$$

where $\bar{R}_\varphi \equiv \sum_q \bar{T}_{\varphi q}$. Inserting $f_\varphi(E)$ into $i_p(E)$:

$$i_p = \frac{2e}{h}\sum_q \bar{T}_{pq}[f_p - f_q] + \frac{2e}{h}\bar{T}_{p\varphi}\left[f_p - \left(\frac{h}{2e}i_\varphi + \sum_q \bar{T}_{\varphi q}f_q\right)/\bar{R}_\varphi\right] \tag{2.139}$$

$$= \frac{2e}{h}(\sum_q \bar{T}_{pq} + \bar{T}_{p\varphi})f_p - \frac{2e}{h}\sum_q\left(\bar{T}_{pq} + \bar{T}_{p\varphi}\frac{\bar{T}_{\varphi q}}{\bar{R}_\varphi}\right)f_q - \frac{\bar{T}_{p\varphi}}{\bar{R}_\varphi}i_\varphi \tag{2.140}$$

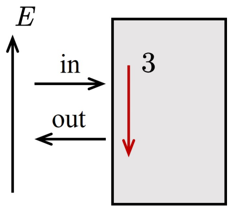
$$= \frac{2e}{h}\left(\sum_q \bar{T}_{pq} + \bar{T}_{p\varphi}\frac{\bar{R}_\varphi}{\bar{R}_\varphi}\right)f_p \cdots \tag{2.141}$$

$$= \frac{2e}{h}\sum_q\left(\bar{T}_{pq} + \frac{\bar{T}_{p\varphi}\bar{T}_{\varphi q}}{\bar{R}_\varphi}\right)f_p - \frac{2e}{h}\sum_q\left(\bar{T}_{pq} + \frac{\bar{T}_{p\varphi}\bar{T}_{\varphi q}}{\bar{R}_\varphi}\right)f_q - \frac{\bar{T}_{p\varphi}}{\bar{R}_\varphi}i_\varphi \tag{2.142}$$

$$= \frac{2e}{h}\sum_q T_{pq}^{eff}[f_p - f_q] - \frac{\bar{T}_{p\varphi}}{\bar{R}_\varphi}i_\varphi \tag{2.143}$$

where $\bar{T}_{pq}^{\text{eff}} = \bar{T}_{pq} + \frac{\bar{T}_{p\varphi}\bar{T}_{\varphi q}}{\bar{R}_\varphi}$.

Note *Floating probe:* $I_p = \int i_p(E)dE = 0$, *not* $i_p(E) = 0$. *In general, decoherence process include inelastic scattering such that electrons are scattered in and out accompanied by energy changes.*



Non-zero $i_\varphi(E)$ is referred to as "vertical flow". Energy non-conserved, incoherent, one should involve exclusion principle. Calculating vertical current needs detailed microscopic theory, beyond the scope of the course.

Complexity: exclusion principle not by $(1 - f)$ factor.

$$f_\varphi(E) \to f_\varphi(r, r', E) \tag{2.144}$$

Drastic assumption: $i_\varphi(E) = 0$, neglecting vertical flow, which actually works well.

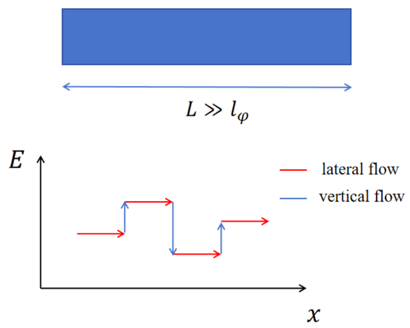
Question: *whether decoherence remains when* $i_\varphi = 0$*?*

Answer: *Yes, even for a fixed energy energy, the inflow and outflow electrons in the virtual probe are different. Some flow to infinity and some are from infinity. Note that the virtual probe is not a part of the scattering region, which extends to infinity.*

2.7 When can we use the Landauer-Büttiker formalism

$$i_p = \frac{2e}{h}\sum_q \overline{T}_{pq}^{eff}[f_p - f_q] - \frac{\overline{T}_{p\phi}}{\overline{R}_\phi} i_\phi \tag{2.145}$$

For Non-coherent elastic transport, $\frac{\overline{T}_{p\phi}}{\overline{R}_\phi} i_\phi = 0$.



One can imagine this picture by the virtual probe, but that is not necessary. The vertical flow is essentially the current non-conservation for the scattering channel of a given energy. Assumption: zero net vertical flow, only phase-breaking, no energy relaxation. Electrons still stay in the same channel, thus there is no Pauli blocking. Landau-Buttiker formula can be used, with the transmission without coherence.

The momentum relaxation and phase breaking dominate mesoscopic transport. For systems with energy relaxation or finite vertical flow, the main effects that determine the resistance are still momentum and phase relaxation. Energy relaxation has no significant impact on the resistance.

2.7.1 Uniform transmission

$\overline{T}(E)$ is independent of energy for μ_2-(a few $k_B T$) $<E<$ μ_1+(a few $k_B T$). Vertical flow has no effect on the resistance, Since all energy channels conduct equally well.

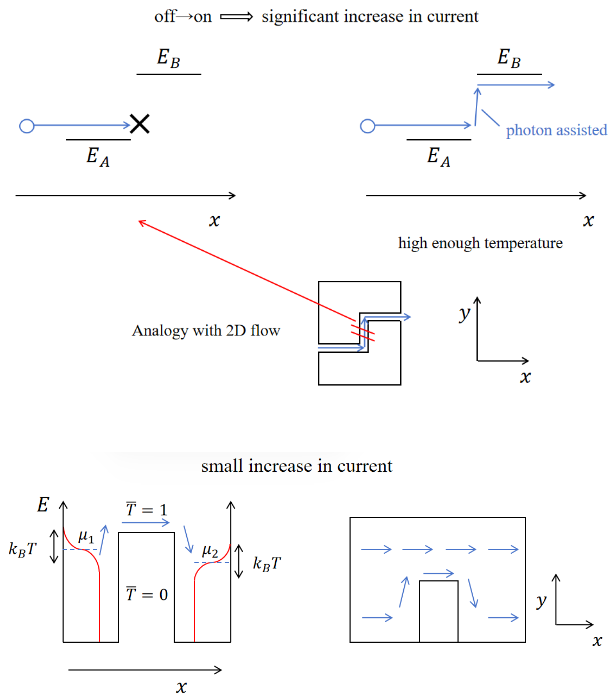
$$i_p = \frac{2e}{h}\sum_q \overline{T}_{pq}^{eff}[f_p - f_q] - \frac{\overline{T}_{p\phi}}{\overline{R}_\phi} i_\phi \tag{2.146}$$

$$I_p = \int i_p(E)dE = \frac{2e}{h}\int \sum_q \overline{T}_{pq}^{eff}[f_p - f_q]dE - \frac{\overline{T}_{p\phi}}{\overline{R}_\phi}\int i_\phi(E)dE \tag{2.147}$$

where the second term is zero (True only for net current, not the energy distribution of current). The heat dissipated $\sim \int E i_\phi(E)dE$ where the vertical flow cannot be neglected.

Summarize: The criterion for neglecting $i_\phi(E)$ is calculating R is $(\mu_1 - \mu_2)+$(a few $k_B T$)$\ll \varepsilon_c$ (correlation energy over which transmission is uniform). Recall regime of linear response: $(\mu_1 - \mu_2) \ll k_B T + \varepsilon_c$, we conclude that zero temperature linear response belongs to the current regime.

2.7.2 Non-uniform transmission



Transport of electrons over a potential barrier.

Remark when inelastic processes exist, LB formalism should be used with caution when the transmission functions vary widely over the energy range of transport. In this regime, decoherence occurs, with $L \gg l_\phi$. In samples with $L < l_\phi$, no inelastic scattering occurs, LB is widely used even if $\overline{T}(E)$ varies strongly. When the response is not linear, we can still use $I = \int i(E)dE, i(E) = \frac{2e}{h}\overline{T}(E)[f_1(E) - f_2(E)]$ for 2-terminal derive. We can define the differential conductance $G_{diff}(E) = \frac{\partial I}{\partial V}$.

Exercise 2.7 (E.2.5, page 115) *Coherent inelastic transport.* In this book we will generally restrict ourselves to steady-state transport in the presence of a d.c. bias. However, it is interesting to note that if an alternating field is present within the conductor (but not inside the contacts) then we can define scattering states just like those in Eq. (2.6.3) but with different energies all coupled together. A scattering state (q, E) now consists of an incident wave with energy E in lead q, together with scattered waves with energy ($E_n = E \pm n\hbar\omega$, n being an integer) in every lead p (cf. Eq. (2.6.3)):

$$\Psi_p(q) = \delta_{pq}\exp[+ikx_q]\exp[-iEt/\hbar] + \sum_{p,n} s'_{pq}(E_n, E)\exp[-ik_n x_p]\exp[-iE_n t/\hbar]$$

Proceeding as before derive the following expression for the *d.c.* current:

$$I_p = \frac{2e}{h}\int\left[f_p(E) - \sum_{q,n} T_{pq}(E_n, E)f_q(E)\right]dE$$

The point is that there is no reason to include any exclusion principle-related factors in the expression for the current even if transport is inelastic, as long as it is coherent. But if there are phase-breaking processes within the conductor then we cannot define coherent scattering states that extend from one lead to another and the scattering state argument cannot be used.

✍ **Exercise 2.8 (E.2.7, page 116)** Starting from the current expression

$$I = \frac{2e}{h} \int \bar{T}(E)[f_1(E) - f_2(E)]dE \qquad \text{(see Eq. (2.5.1))}$$

derive the result stated in Eqs. (2.5.4)-(2.5.6) (see P. F. Bagwell and T. P. Orlando (1989), *Phys. Rev. B*, **40**, 1456).

Chapter 3 Scattering Approach

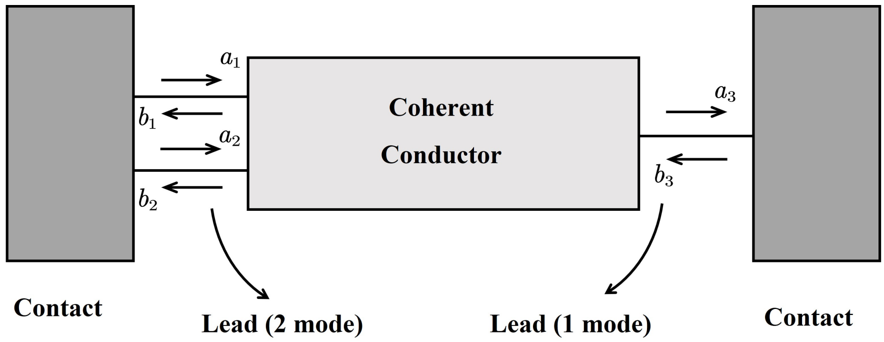
3.1 Transmission function and the S-matrix

The LB method expresses the current in terms of the transmission function. For coherent conductors, the transmission functions are obtained by the scattering matrix (S-matrix).

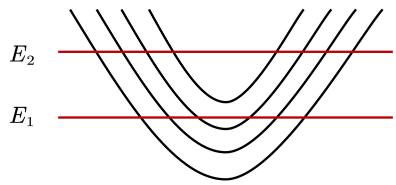
A coherent conductor can be characterized at each energy by an S-matrix that relates the outgoing wave amplitude to the incoming wave amplitudes in all leads.

$$\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \tag{3.1}$$

where b_i represents the amplitude of the outgoing wave, while a_i represents the amplitude of the incident wave.



For a given energy E, the number of modes at lead p is denoted by $M_p(E)$, which is a function of E, then the total number of modes is given by $M_T(E) = \sum_p M_p(E)$. Thus, the dimensions of S-matrix is given by $M_T \times M_T$, in general, it contains two labels, p, n, meaning channel n is lead p.



Remark The incoming and outgoing channels should have the same number.

Transmission probability:

$$T_{pn,qm} = T_{pn \leftarrow qm} = |S_{pn,qm}|^2, \qquad S_{pn,qm} = S_{pn \leftarrow qm} \tag{3.2}$$

where qm represents the mode m in lead q, and pn represents the mode n in lead p. Thus the transmission function between different leads is given by:

$$\bar{T}_{pq} = \sum_{m \in q} \sum_{n \in p} T_{pn,qm} \tag{3.3}$$

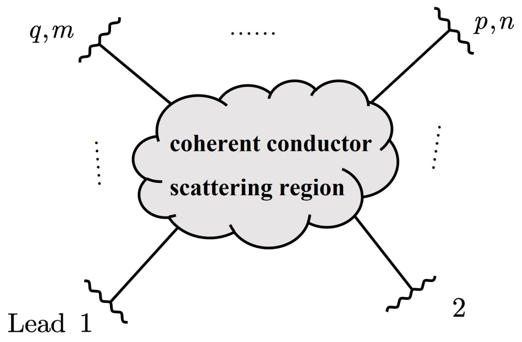
Calculate the S-matrix in is the main task for the transport problem of a coherent conductor. We first analyze the properties of S-matrix with its general form.

A general incoming state, superposition of different incident modes

$$\Psi^{(in)} = \sum_{qm} a_{qm} \psi_{qm}^{(in)} \tag{3.4}$$

Similarly, the outgoing state is

$$\Psi^{(out)} = \sum_{pn} a_{pn} \psi_{pn}^{(out)} \tag{3.5}$$



For a scattering problem, we aim to find the outgoing amplitudes $\{b_{pn}\}$ for the incoming amplitudes $\{a_{qm}\}$. Assume that only one channel injects electron (let's assume lead 1, without loss of generality):

$$\psi_{q1}^{(in)} \Rightarrow \psi_{q1}^{(out)} = \sum_{pn} S_{pn,q1} \psi_{pn}^{(out)} \tag{3.6}$$

where $S_{pn,q1}$ is the scattering amplitude. This corresponds to the typical example of scattering problem is $\langle\langle QM \rangle\rangle$. Now use the superposition principle for a general incident state $\psi^{(in)} = \sum_{qm} a_{qm} \psi_{qm}^{(in)}$, the outgoing state is:

$$\Psi_{q1}^{(in)} \Rightarrow \Psi_{q1}^{(out)} = \sum_{qm} a_{qm} \Psi_{qm}^{(out)} = \sum_{qm} a_{qm} \sum_{pn} S_{pn,qm} \psi_{pn}^{(out)} \tag{3.7}$$

$$= \sum_{pn} b_{pn} \psi_{pn}^{(out)} \tag{3.8}$$

$$\Rightarrow b_{pn} = \sum_{qm} S_{pn,qm} a_{qm} \iff \{b\} = [S]\{a\} \tag{3.9}$$

where $\{a\} = (a_1, a_2, ...)^T$, and $\{b\} = (b_1, b_2, ...)^T$. These relations are general properties of S-matrix.

3.1.1 Unitarity: current conservation

Current conservation:

$$\sum_{qm} |a_{qm}|^2 = \sum_{pn} |b_{pn}|^2 \iff \{a\}^\dagger \{a\} = \{b\}^\dagger \{b\} \tag{3.10}$$

$\{a_{qm}, b_{pn}\}$: normalized current amplitudes $=$ wave amplitudes $\times \sqrt{v_{out}/v_{in}}$. [1]

Substitute the S-matrix into Eq. (3.10):

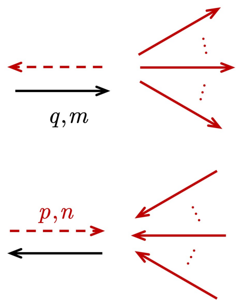
$$\{a^\dagger\}\{a\} = \{a\}^\dagger [S]^\dagger [S] \{a\} \tag{3.11}$$

$$\Rightarrow [S]^\dagger [S] = I = [S][S^\dagger] = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \ddots \end{pmatrix} \tag{3.12}$$

$$[S^\dagger S]_{pn,qm} = \sum_{\alpha l} S_{pn,\alpha l}^\dagger S_{\alpha l,qm} = \sum_{\alpha l} S_{\alpha l,pn}^* S_{\alpha l,qm} = \delta_{pq}\delta_{mn} \tag{3.13}$$

- For $p = q, m = n$, $\sum_{\alpha l} |S_{\alpha l,qm}|^2 = \sum_{\alpha l} T_{\alpha l,qm} = 1$. The outgoing current equals the incident current in q, m current conservation.
- For $p \neq q$, or $m \neq n$, $\sum_{\alpha l} S_{pn,\alpha l}^\dagger S_{\alpha l,qm} = \sum_{\alpha l} S_{\alpha l,pn}^* S_{\alpha l,qm} = 0$.

[1] Current conservation, rather than |amplitude|^2 conservation!



Similarly, $[SS^\dagger]_{pn,qm} = \delta_{pq}\delta_{mn} = \sum_{\alpha l} S_{pn,\alpha l} S^\dagger_{\alpha l,qm} = \sum_{\alpha l} S_{pn,\alpha l} S^*_{qm,\alpha l}$, thus $\sum_{\alpha l} |S_{pn,\alpha l}|^2 = \sum_{\alpha l} T_{pn,\alpha l} = 1$.

3.1.2 Sum rules

Recall transmission function $\bar{T}_{pq} = \sum_{m\in q}\sum_{n\in p} T_{pn,qm}$. Now we have using the unitarity of the S-matrix:

$$\sum_q \bar{T}_{pq} = \sum_q \sum_{m\in q} \sum_{n\in p} T_{pn,qm} = \sum_{n\in p} (\sum_{qm} T_{pn,qm}) = \sum_{n\in p} 1 = M_p \tag{3.14}$$

$$\sum_p \bar{T}_{pq} = \sum_p \sum_{m\in q} \sum_{n\in p} T_{pn,qm} = \sum_{m\in q} (\sum_{pn} T_{pn,qm}) = \sum_{m\in q} 1 = M_q \tag{3.15}$$

therefore, we can derive the relation we previously used[2]:

$$\sum_q \bar{T}_{pq}(E) = \sum_q \bar{T}_{qp}(E) = M_p(E) \tag{3.16}$$

Matrix of transmission function $N \times N$, N leads, for $N = 3$:

$\bar{T}_{pq}(E)$	q=1	2	3	SUM
p=1	$\bar{T}_{11}(E)$	$\bar{T}_{12}(E)$	$\bar{T}_{13}(E)$	M_1
2	$\bar{T}_{21}(E)$	$\bar{T}_{22}(E)$	$\bar{T}_{23}(E)$	M_2
3	$\bar{T}_{31}(E)$	$\bar{T}_{32}(E)$	$\bar{T}_{33}(E)$	M_3
SUM	M_1	M_2	M_3	

Special case: 2-terminal ⇒reciprocal (even with B):

$\bar{T}_{pq}(E)$	q=1	2	SUM
p=1	$\bar{T}_{11}(E)$	$\bar{T}_{12}(E)$	M_1
2	$\bar{T}_{21}(E)$	$\bar{T}_{22}(E)$	M_2
3	$\bar{T}_{31}(E)$	$\bar{T}_{32}(E)$	M_3
SUM	M_1	M_2	

$$\bar{T}_{11} + \bar{T}_{12} = M_1 = \bar{T}_{11} + \bar{T}_{21} \Rightarrow \bar{T}_{21} = \bar{T}_{12} \tag{3.17}$$

Sum rule for conductance matrix

$$\sum_q G_{qp} = \sum_q G_{pq} = \frac{2e^2}{h}\int \sum_q \bar{T}_{pq}(E)(-\frac{\partial f_0}{\partial E})dE = \frac{2e^2}{h}\int M_p(E)(-\frac{\partial f_0}{\partial E})dE \simeq \frac{2e^2}{h} M_p(E_F) \tag{3.18}$$

In the linear response regime, the unitarity of the S-matrix ensures the sum rule for the conductance matrix.

[2] Sum over one subscript, equals the number of modes in the lead labeled by the other subscript.

3.1.3 Symmetry properties of S-matrix

Note *S-matrix is determined by the dynamics of the system. The dynamics is governed by the Hamiltonian of the system. If the system processes certain symmetry, mathematically, this means certain constraint on the Hamiltonian. Accordingly, it also imposes constraint on the dynamics of the system, or, the symmetry of the Hamiltonian will be inherited by the dynamics and the S-matrix.*

Here, we focus on two non-spatial symmetries, which do not rely on the crystalline symmetries and thus can be widely applied.

3.1.3.1 Time-reversal symmetry

Time-reversal symmetry: $H^* = H \Rightarrow S^\dagger = S$ (spin degenerate case).

Schrödinger equation:

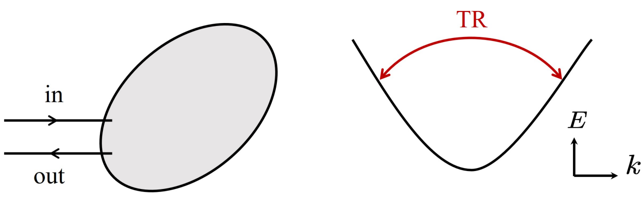
$$i\hbar\frac{\partial\Psi(t)}{\partial t} = H\Psi(t) \tag{3.19}$$

Time reversal $t \to -t$:

$$\Rightarrow -i\hbar\frac{\partial\Psi(-t)}{\partial t} = H\Psi(-t) \tag{3.20}$$

$$\text{(complex conjugate)} \quad \Rightarrow i\hbar\frac{\partial\Psi^*(-t)}{\partial t} = H^*\Psi^*(-t) = H\Psi^*(-t) \tag{3.21}$$

where $H^*\Psi^*(-t) = H\Psi^*(-t)$ indicate the Time-reversal symmetry, we see $\Psi^*(-t)$, $\Psi(t)$ satisfy the same equation.



This will impose nontrivial constraint on the S-matrix, because TR operation switches the incoming and outgoing states are each other's TR-counterpart:

$$\psi^{(in)}(t) = \exp\left[ikx + \frac{E}{i\hbar}t\right] \tag{3.22}$$

$$\psi^{(out)}(t) = \exp\left[-ikx + \frac{E}{i\hbar}t\right] \tag{3.23}$$

We see that $\psi^{(out)}(-t)^* = \psi^{(in)}(t)$[3].

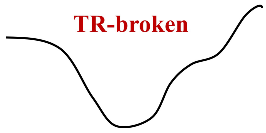
Use $\psi^{(out)}(-t)^*$ to express incoming state, $\psi^{(in)}(-t)^*$ to express outgoing state:

$$\Psi^{(in)}(t) = \sum_{qm} a_{qm}\psi^{(in)}_{qm}(t) \Rightarrow \Psi^{(out)}_{new}(t) = [\Psi^{(in)}(-t)]^* = \sum_{qm} a^*_{qm}\psi^{(in)}_{qm}(-t)^* = \sum_{qm} a^*_{qm}\psi^{(out)}_{qm}(t) \tag{3.24}$$

$$\Psi^{(out)}(t) = \sum_{pn} a_{pn}\psi^{(out)}_{pn}(t) \Rightarrow \Psi^{(in)}_{new}(t) = [\Psi^{(out)}(-t)]^* = \sum_{pn} b^*_{pn}\psi^{(out)}_{pn}(-t)^* = \sum_{pn} b^*_{pn}\psi^{(in)}_{pn}(t) \tag{3.25}$$

[3] complex conjugate: $k \to -k$, $-t \to t$, which means the exchange of (in) $\leftrightarrow$ (out).

Here, TR symmetry is reflected in two aspects:



(a) $\psi^{(in)}(E)$, $\psi^{(out)}(E)$ are TR partners and exchange roles in the scattering problem:

$$\psi^{(in)} \leftrightarrow \psi^{(out)*}, \qquad \{a\} \leftrightarrow \{b\}^* \tag{3.26}$$

(b) Schrödinger equation remains the same.

Note that the S-matrix is solved by SEQ + boundaries, meaning that

$$\begin{cases} \{b\} = [S]\{a\} \\ \{a\}^* = [S]\{b\}^* \Rightarrow [S]^\dagger\{a\}^* = \{b\}^* \Rightarrow \{b\} = [S]^T\{a\} \end{cases} \Rightarrow \qquad [S] = [S]^\dagger \tag{3.27}$$

This is for the spin degenerate case. For the spin dependent case, revision is needed.

In particular, for topological surface states with spin-momentum locking, the TRS requires $[S] = -[S]^T$ [4]. With B reciprocity, $[S]_B = [S^T]_{-B}$.

This is equivalent to the TRS as we involve B in the H, and require B to be inverted under TR operation. In particular

$$[E_s + \frac{(i\hbar\nabla + e\vec{A})^2}{2m} + U(x,y)]\Psi_B(x,y) = E\Psi_B(x,y), \qquad \text{TR} + \vec{A} \to -\vec{A} \tag{3.28}$$

$$\Rightarrow [E_s + \frac{(i\hbar\nabla + e\vec{A})^2}{2m} + U(x,y)]\Psi_B^*(x,y) = E\Psi_B^*(x,y) \tag{3.29}$$

3.1.3.2 Particle-hole symmetry (Superconductor-Hybridized system)

We need three steps: (i) PH symmetry of H_{BdG}. (ii) Its implication for the spectrum and states. (iii) PH symmetry of S-matrix. (iv) BTK formula.

3.1.3.3 Bogoliubov-de Gennes (BdG) equation, or Nambu representation

When the system contains a superconductor, the $U(1)$ gauge symmetry is broken. It is convenient to interpret the system in the language of electron-hole, or using Bogoliubov-de Gennes Hamiltonian. The corresponding spinor is called Nambu spinor. For a BCS Hamiltonian

$$H_{BCS} = \int d\vec{r} \left\{ \sum_{\sigma\sigma'} \left(\psi_\sigma^\dagger(r) H_{\sigma\sigma'}(r)\psi_{\sigma'}(r) \right) + \Delta(r)\psi_\uparrow^\dagger(r)\psi_\downarrow^\dagger(r) + \Delta^*(r)\psi_\downarrow(r)\psi_\uparrow(r) \right\} \tag{3.30}$$

the normal part is generally expressed by

$$H = H_{N,D} + H_Z + H_R \tag{3.31}$$

$$H_N = \frac{p^2}{2m} + V(\vec{r}) - \mu \qquad \text{normal electron} \tag{3.32}$$

$$H_D = \hbar v_D \vec{\sigma}\vec{p} + V(\vec{r}) - \mu \qquad \text{Dirac electron} \tag{3.33}$$

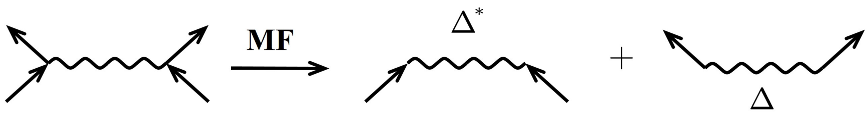
$$H_Z = \frac{1}{2} g\mu_B \vec{B}\vec{\sigma} \qquad \text{Zeeman splitting} \tag{3.34}$$

$$H_R = \alpha\vec{\sigma} \times \vec{p} \cdot \hat{z} \qquad \text{Rashba SOC} \tag{3.35}$$

where $V(\vec{r})$ is the electric potential, μ is the chemical potential, g is the Landé factor, and Δ is the pair potential.

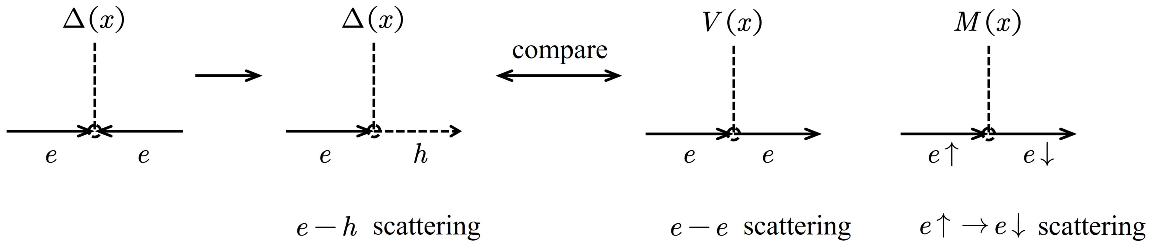
BCS Hamiltonian is a many-body Hamiltonian, involving operators like $\psi^\dagger\psi^\dagger$, $\psi\psi$. After mean-field approximation, the number of electrons is unconserved.

[4] Reference: Bardarso, Moore, Rep. Prog. phys 76, 056501 (2013)



By interpreting half of electrons as holes, the physical picture of $e-e$ interaction is transferred into $e \to h$ scattering, similar to $e \to e$ scattering[5].

Particle-hole transformation: $\psi_\sigma \leftrightarrow \psi^\dagger_{\bar{\sigma}h}$, annihilation of an electron with spin σ is equivalent to creation of a hole with spin $\bar{\sigma}$.



Mathematically, this is equivalent to the "spin flipped" scattering

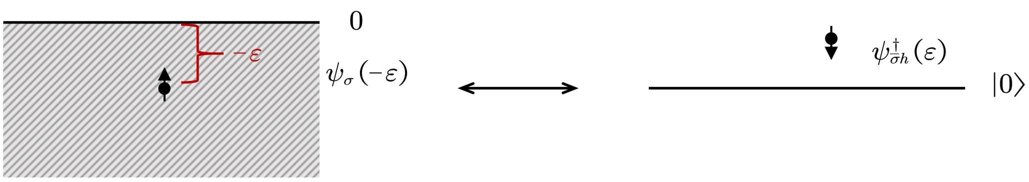
$$\frac{1}{2}\Delta(r)\psi^\dagger_\uparrow(r)\psi^\dagger_\downarrow(r) \to \frac{1}{2}\Delta(r)\psi^\dagger_\uparrow(r)\psi_{\uparrow,h}(r) \tag{3.36}$$

$$\Longleftrightarrow\ -\frac{1}{2}\Delta(r)\psi^\dagger_\downarrow(r)\psi^\dagger_\uparrow(r) \to -\frac{1}{2}\Delta(r)\psi^\dagger_\downarrow(r)\psi_{\downarrow,h}(r) \tag{3.37}$$

$$\frac{1}{2}\Delta^*(r)\psi_\downarrow(r)\psi_\uparrow(r) \to \frac{1}{2}\Delta^*(r)\psi^\dagger_{\uparrow,h}(r)\psi_\uparrow(r) \tag{3.38}$$

$$\Longleftrightarrow\ -\frac{1}{2}\Delta^*(r)\psi_\uparrow(r)\psi_\downarrow(r) \to \frac{1}{2}\Delta^*(r)\psi^\dagger_{\downarrow,h}(r)\psi_\downarrow(r) \tag{3.39}$$

In the $e-h$ language, the $e-h$ scattering is spin conserved (we assume spin-singlet pairing here) but charge unconserved, consistent with the full electron language, $\psi_\uparrow\psi_\downarrow$, $\psi^\dagger_\uparrow\psi^\dagger_\downarrow$.



energy ε measured from μ

In the Nambu space, $\Delta(r)$, $\Delta^*(r)$ are off-diagonal parts. For the diagonal parts, we have H_N, H_D for the electron part. We also need to interpart half of electrons as holes, that is

$$\psi^\dagger_\sigma H_{\sigma\sigma'}\psi_{\sigma'} \to \frac{1}{2}\psi^\dagger_\sigma H_{\sigma\sigma'}\psi_{\sigma'} + \frac{1}{2}\psi^\dagger_{\sigma,h}H^h_{\sigma\sigma'}\psi_{\sigma',h} \tag{3.40}$$

[5]Price: double dimension of Hilbert space.

specifically, for normal electron

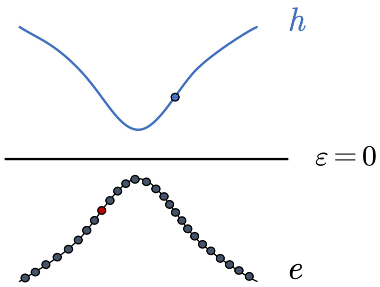
$$\sum_\sigma \int d\vec{r}\psi^\dagger_\sigma(r)H_N(r)\psi_\sigma(r) = \sum_\sigma \int d\vec{r}\psi^\dagger_\sigma(r)\left[\frac{p^2}{2m}+V(r)-\mu\right]\psi_\sigma(r) \tag{3.41}$$

$$= \sum_\sigma \int d\vec{r}\psi_\sigma(r)\left[-\frac{p^2}{2m}-V(r)+\mu\right]\psi^\dagger_\sigma(r) + \text{const} \tag{3.42}$$

$$= \sum_\sigma \int d\vec{r}\psi^\dagger_{\bar{\sigma},h}(r)H_N(r)\psi_{\bar{\sigma},h}(r) \tag{3.43}$$

$$\Rightarrow H^h_N(r) = -H_N(r) \tag{3.44}$$

Remark Physical meaning, the entire Fermi sea with the absence of one electron with energy $-\varepsilon$, spin $\uparrow$, momentum k, can be effectively described by a single hole with energy ε, spin $\downarrow$, momentum $-k$, because the entire Fermi sea has energy 0, spin 0. The particle-hole transformation is the same as that in semiconductor.



$$c_\uparrow(k,\varepsilon) \leftrightarrow c^\dagger_{\downarrow h}(-k,-\varepsilon)$$

For the diagonal part, if the Hamiltonian is spin-dependent, then H^h dose not differ for H by a minus sign. For the Dirac fermion, or Rashba SOC, we have the following form:

$$\int d\vec{r}\,\psi^\dagger_\sigma(r)\nabla\psi_{\sigma'}(r) = \int d\vec{r}\,\psi_{\sigma'}(r)\nabla\psi^\dagger_\sigma(r) + \cancel{\text{const}} = \int d\vec{r}\,\psi_{\sigma'}(r)\nabla\psi^\dagger_\sigma(r) \tag{3.45}$$

Proof

$$\int d\vec{r}\,\psi^\dagger_\sigma(r)\nabla\psi_{\sigma'}(r) = \sum_{kk'}\int d\vec{r}\,e^{-ikr}c^\dagger_{k\sigma}\nabla e^{ik'r}c_{k'\sigma'} \tag{3.46}$$

$$= \sum_{kk'}\int d\vec{r}\,e^{-i(k-k')r}(ik')c^\dagger_{k\sigma}c_{k'\sigma'} = \sum_{kk'}\delta_{kk'}ik'c^\dagger_{k\sigma}c_{k'\sigma'} \tag{3.47}$$

$$= \sum_{kk'}\delta_{kk'}ik(-c_{k'\sigma'}c^\dagger_{k\sigma}) + \cancel{\sum_k ik\delta_{\sigma\sigma'}} \tag{3.48}$$

$$= \sum_{kk'}\delta_{kk'}(-ik)c_{k'\sigma'}c^\dagger_{k\sigma} = \sum_{kk'}\int d\vec{r}\,e^{-i(k-k')r}(-ik)c_{k'\sigma'}c^\dagger_{k\sigma} \tag{3.49}$$

$$= \sum_{kk'}\int d\vec{r}\,(\nabla e^{-ikr})e^{ik'r}c_{k'\sigma'}c^\dagger_{k\sigma} \tag{3.50}$$

$$= \int d\vec{r}\,\psi_{\sigma'}(r)\nabla\psi^\dagger_\sigma + \text{const} = \int d\vec{r}\,\psi^\dagger_{\bar{\sigma}'h}(r)\nabla\psi_{\bar{\sigma}h}(r) \tag{3.51}$$

As such, the full BdG Hamiltonian can be obtained.

Two commonly use Nambu representation:

$$\Phi_1 = (\psi_\uparrow, \psi_\downarrow, \psi^\dagger_\uparrow, \psi^\dagger_\downarrow), \qquad \Phi_2 = (\psi_\uparrow, \psi_\downarrow, \psi^\dagger_\downarrow, -\psi^\dagger_\uparrow) \tag{3.52}$$

$\vec{k}$-representation:

$$\Phi^k_1 = (c_{k\uparrow}, c_{k\downarrow}, c^\dagger_{-k\uparrow}, c^\dagger_{-k\downarrow}), \qquad \Phi^k_2 = (c_{k\uparrow}, c_{k\downarrow}, c^\dagger_{-k\downarrow}, c^\dagger_{-k\uparrow}) \tag{3.53}$$

The form of the BdG Hamiltonian depends on the representation, but the physical results should not.

$$\Phi_1 : H^1_{BdG} = \frac{1}{2}\begin{bmatrix} H & i\sigma_y\Delta \\ -i\sigma_y\Delta^* & -H^* \end{bmatrix} \quad \Phi_2 : H^2_{BdG} = \frac{1}{2}\begin{bmatrix} H & \Delta \\ \Delta^* & -THT^{-1} \end{bmatrix} \tag{3.54}$$

where $T = i\sigma k$ is the time-reversal operator.

The BdG Hamiltonian interprets the system as half-electron, half-hole. Mathematically, such interpretation impose constraint on the BdG Hamiltonian, termed as particle-hole symmetry. We have

$$(\Phi_1^\dagger)^T = \hat{\tau}_x\Phi_1 \quad (\Phi_2^\dagger)^T = \sigma_y\tau_y\Phi_2 \tag{3.55}$$

where $\tau_{x,y}$ is the Pauli matrices in Nambu space, and $\hat{\tau}_{x,y} = \tau_{x,y} \otimes \mathbb{1}$. Substituting the above expression with specific matrices yields:

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \\ \psi_\uparrow^\dagger \\ \psi_\downarrow^\dagger \end{pmatrix} = \begin{pmatrix} \psi_\uparrow^\dagger \\ \psi_\downarrow^\dagger \\ \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = (\Phi_1^\dagger)^T \qquad \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \\ \psi_\downarrow^\dagger \\ -\psi_\uparrow^\dagger \end{pmatrix} = \begin{pmatrix} \psi_\uparrow^\dagger \\ \psi_\downarrow^\dagger \\ \psi_\downarrow \\ -\psi_\uparrow \end{pmatrix} = (\Phi_2^\dagger)^T \tag{3.56}$$

It can be proved that the BdG Hamiltonian satisfies the particle-hole symmetry.

$$\{\Xi_i, H^i_{BdG}\} = 0 \tag{3.57}$$

$\Xi_1 = \tau_x K$, $\Xi_2 = \sigma_y\tau_y K$, are the symmetry operators in the corresponding representation. Again, the symmetry operations depend on representation. The particle-hole transformation operator is anti-unitary.

Proof of $\{\Xi_1, H^1_{BdG}\} = 0$ for representation Φ_1, drop subscript $i = 1$:

Proof

$$\hat{H}_{BdG} = \Phi^\dagger H\Phi = \sum_{i,j=\{\sigma,\tau\}} \Phi_i^\dagger H_{ij}\Phi_j = \sum_{ij}(\hat{\tau}_x\Phi)_i H_{ij}(\Phi^\dagger\hat{\tau}_x)_j \tag{3.58}$$

$$= \sum_{ij}\sum_{kl}\tau_x^{ik}\Phi_k H_{ij}\Phi_l^\dagger\tau_x^{lj} = \sum_{ijkl}\tau_x^{ik}H_{ij}\tau_x^{lj}\Phi_k\Phi_l^\dagger \tag{3.59}$$

$$= \sum_{ijkl}\tau_x^{ik}H_{ij}\tau_x^{lj}(\delta_{kl} - \Phi_l^\dagger\Phi_k) = \sum_{ijkl}\Phi_l^\dagger(-\tau_x^{ik}H_{ij}\tau_x^{lj})\Phi_k + \sum_{ijk}\tau_x^{ik}H_{ij}\tau_x^{kj} \tag{3.60}$$

$$= \sum_{ijkl}\Phi_l^\dagger(-\tau_x^{lj}H_{ji}^*\tau_x^{ik})\Phi_k + \frac{1}{2}\sum_{ijk}\tau_x^{kj}H_{ji}^*\tau_x^{ik} + \frac{1}{2}\sum_{ijk}\tau_x^{ki}H_{ij}\tau_x^{jk} \tag{3.61}$$

$$= \sum_{kl}\Phi_l^\dagger(-\tau_x H^*\tau_x)_{lk}\Phi_k + \frac{1}{2}\mathrm{Tr}[\tau_x(H + H^*)\tau_x] \tag{3.62}$$

$$= \Phi^\dagger(-\tau_x H^*\tau_x)\Phi \tag{3.63}$$

$$\Rightarrow \Phi^\dagger H\Phi = \Phi^\dagger(-\tau_x H^*\tau_x)\Phi \Rightarrow H = -\tau_x H^*\tau_x = \Xi_1 H\Xi_1^{-1} \Rightarrow \{\Xi_1, H^1_{BdG}\} = 0 \tag{3.64}$$

$$\mathrm{Tr}[\tau_x H^* + H]\tau_x = \mathrm{Tr}\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} H_{11}+H_{11}^* & H_{12}+H_{12}^* \\ H_{21}+H_{21}^* & H_{22}+H_{22}^* \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] \tag{3.65}$$

$$= \mathrm{Tr}\left[\begin{pmatrix} H_{21}+H_{21}^* & H_{22}+H_{22}^* \\ H_{11}+H_{11}^* & H_{12}+H_{12}^* \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] \tag{3.66}$$

$$= \mathrm{Tr}\left[\begin{pmatrix} H_{22}+H_{22}^* & H_{21}+H_{21}^* \\ H_{12}+H_{12}^* & H_{11}+H_{11}^* \end{pmatrix}\right] \tag{3.67}$$

$$= H_{11}+H_{11}^*+H_{22}+H_{22}^* \tag{3.68}$$

$$= H + H^* - H^* - H = 0 \tag{3.69}$$

Remark The symmetry is expressed by the anti-commutation relation rather than the commutation such as the time-reversal symmetry, $[T, H] = 0$.

Exercise 3.1 Prove that:

$$\sum_{ijk} \tilde{\tau}_x^{ik} H_{BdG}^{ij} \tilde{\tau}_x^{kj} = 0$$

where $\tilde{\tau}_x = \sigma_0 \otimes \tau_x$, and H_{BdG} is the BdG Hamiltonian in basis $\Phi = (\psi_\uparrow, \psi_\downarrow, \psi_\uparrow^\dagger, \psi_\downarrow^\dagger)^T$:

$$H_{BdG} = \frac{1}{2}\begin{pmatrix} H & i\sigma_y\Delta \\ -i\sigma_y\Delta^* & -H^* \end{pmatrix}$$

Solution *Note that $\tilde{\tau}_x = \tilde{\tau}_x^T$, then:*

$$\sum_{ijk} \tilde{\tau}_x^{ik} H_{BdG}^{ij} \tilde{\tau}_x^{kj} = \frac{1}{2}\sum_{ijk}\left[\tilde{\tau}_x^{ki} H_{BdG}^{ij} \tilde{\tau}_x^{jk} + \tilde{\tau}_x^{kj} {H_{BdG}^{ji}}^* \tilde{\tau}_x^{ik}\right]$$

$$= \frac{1}{2}\mathrm{Tr}\left[\tilde{\tau}_x (H_{BdG} + H_{BdG}^*)\tilde{\tau}_x\right]$$

$$= \frac{1}{2}\mathrm{Tr}\left[\tilde{\tau}_x\tilde{\tau}_x (H_{BdG} + H_{BdG}^*)\right]$$

$$= \frac{1}{2}\mathrm{Tr}\left[H_{BdG} + H_{BdG}^*\right]$$

$$= \frac{1}{2}\left[H - H^* + H^* - H\right] = 0$$

Exercise 3.2 At the interface between the normal metal and the superconductor, Andreev reflection may occur. The BdG equation can be written as:

$$i\hbar\partial_t \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} -\frac{\hbar^2\nabla^2}{2m} - \mu(x) + V(x) & \Delta(x) \\ \Delta^*(x) & \frac{\hbar^2\nabla^2}{2m} + \mu(x) - V(x) \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix}$$

where $\Delta(x) = \theta(x)\Delta$ and $V(x) = H\delta(x)$. Solve the scattering coefficient of this scattering problem.

Hint: use plane-wave ansatz:

$$\begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix} e^{i(kx - Et/\hbar)} \tag{3.70}$$

then solve the stationary eigenvalue equation and apply the boundary condition at $x = 0$.

Solution *BdG equation:*

$$i\hbar\partial_t \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} -\frac{\hbar^2\nabla^2}{2m} - \mu(x) + V(x) & \Delta(x) \\ \Delta^*(x) & \frac{\hbar^2\nabla^2}{2m} + \mu(x) - V(x) \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} \tag{3.71}$$

plane-wave ansatz:

$$\begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix} e^{i(kx - Et/\hbar)} \tag{3.72}$$

then solve the stationary eigenvalue equation:

$$\begin{pmatrix} -\frac{\hbar^2\nabla^2}{2m} - \mu(x) & \Delta(x) \\ \Delta^*(x) & \frac{\hbar^2\nabla^2}{2m} + \mu(x) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix} \tag{3.73}$$

for normal metal ($x < 0$):

$$\begin{cases} u_0 = 1 - v_0 = 0 \text{ or } 1 \\ \hbar q^\pm = \sqrt{2m}\sqrt{\mu \pm E} \end{cases} \tag{3.74}$$

for a superconductor ($x > 0$), when $E > \Delta$:

$$\begin{cases} u_0 = \sqrt{\frac{\Delta}{2E}} e^{\frac{1}{2}\cosh^{-1}\frac{E}{\Delta}} \\ v_0 = \sqrt{\frac{\Delta}{2E}} e^{-\frac{1}{2}\cosh^{-1}\frac{E}{\Delta}} \\ \hbar k^\pm = \sqrt{2m}\sqrt{\mu \pm (E^2 - \Delta^2)^{1/2}} \end{cases} \tag{3.75}$$

and when $E < \Delta$:

$$\begin{cases} u_0 = \sqrt{\frac{\Delta}{2E}} e^{\frac{i}{2}\cosh^{-1}\frac{E}{\Delta}} \\ v_0 = \sqrt{\frac{\Delta}{2E}} e^{-\frac{i}{2}\cosh^{-1}\frac{E}{\Delta}} \\ \hbar k^\pm = \sqrt{2m}\sqrt{\mu \pm i(\Delta^2 - E^2)^{1/2}} \end{cases} \tag{3.76}$$

Then the scattering state can be expressed by:

$$\psi_N = \frac{1}{\sqrt{2\pi\hbar v}} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{iq^+x} + r_{he} \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{iq^-x} + r_{ee} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-iq^+x} \right] \qquad \textit{for Normal metal } x < 0 \tag{3.77}$$

$$\psi_S = \frac{1}{\sqrt{2\pi\hbar(u_0^2 - v_0^2)v}} \left[t_{ee} \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} e^{ik^+x} + t_{he} \begin{pmatrix} v_0 \\ u_0 \end{pmatrix} e^{-ik^-x} \right] \qquad \textit{for Superconductor } x > 0 \tag{3.78}$$

where $v = \sqrt{2\mu/m}$ is the velocity in normal metal, and assuming $E_F \equiv \mu \gg \Delta$, it follows that $k^\pm \simeq q^\pm \simeq k_F$.

The boundary condition can be derived from the stationary eigenvalue equation at the interface:

$$\begin{pmatrix} -\frac{\hbar^2\nabla^2}{2m} - \mu(x) + V(x) & \Delta(x) \\ \Delta^*(x) & \frac{\hbar^2\nabla^2}{2m} + \mu(x) - V(x) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}$$

$$\Rightarrow \begin{cases} \left[-\frac{\hbar^2\nabla^2}{2m} - \mu(x) + V(x)\right] u(x) + \Delta(x)v(x) = Eu(x) \\ \Delta^*(x)u(x) + \left[\frac{\hbar^2\nabla^2}{2m} + \mu(x) - V(x)\right] v(x) = Ev(x) \end{cases}$$

considering the continuity of the wavefunction and integral the above equation from $x = 0^-$ to $x = 0^+$:

$$\begin{cases} \psi_S(0) = \psi_N(0) = \psi(0) & \textit{continuity} \\ \psi_S'(0) - \psi_N'(0) = \frac{2mH}{\hbar^2}\psi(0) & \textit{discontinuity} \end{cases}$$

By substituting $\psi_{S/N}$ into the boundary condition, the scattering parameter can be obtained:

$$
\begin{aligned}
r_{ee} &= \frac{Z^2 + iZ(v_0^2 - u_0^2)}{u_0^2 + Z^2(u_0^2 - v_0^2)} \\
r_{he} &= \frac{u_0 v_0}{u_0^2 + Z^2(u_0^2 - v_0^2)} \\
t_{ee} &= \frac{(1 - iZ)u_0\sqrt{u_0^2 - v_0^2}}{u_0^2 + Z^2(u_0^2 - v_0^2)} \\
t_{he} &= \frac{iZv_0\sqrt{u_0^2 - v_0^2}}{u_0^2 + Z^2(u_0^2 - v_0^2)}
\end{aligned}
$$

where $Z = H/(\hbar v)$.

Another symmetry called *Chiral symmetry*, is defined as follows: there is a unitary operator that anti-commutes with the Hamiltonian

$$\{U, H\} = 0 \tag{3.79}$$

Comparison between three non-spatial symmetries:

Symms	TR	PH	Chiral
Operators	anti-unitary	anti-unitary	unitary
Forms	commutation	anti-commutation	anti-commutation
Operation	$(k,\uparrow) \to (-k,\downarrow)$	$(k,\uparrow) \to (-k,\downarrow)$	$(k,\uparrow) \to (k,\uparrow)$
...	$E \to E$	$E \to E$	$E \to -E$
Spectrum	Kramers degeneracy	$\{E, -E\}$	$\{E, -E\}$

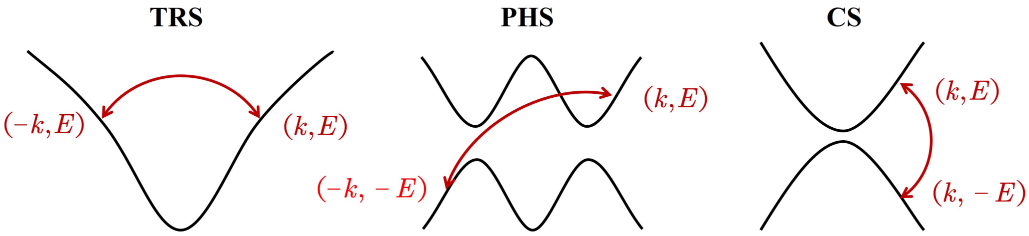
3.1.4 Symmetric energy spectrum[6]

Considering eigenvalue equation:

$$H_{BdG}\chi^i(E_i) = E_i\chi^i(E_i) \tag{3.80}$$

$$\Rightarrow \Xi H_{BdG}\Xi^{-1}\Xi\chi^i(E_i) = E_i\Xi\chi^i(E_i) \tag{3.81}$$

Use $\{\Xi, H_{BdG}\} = 0$, we obtain that $\Xi\chi^i(E_i) = -E_i\Xi\chi^i(E_i)$, so that $\Xi\chi^i(E_i)$ is an eigenstate of H_{BdG}, with eigenenergy $-E_i$.



Remark Symmetry means constraint, which always has nontrivial results. Here, the P-H symmetry is somehow artificial, because we regard half the electrons as holes. As a result, such a symmetry is redundant.

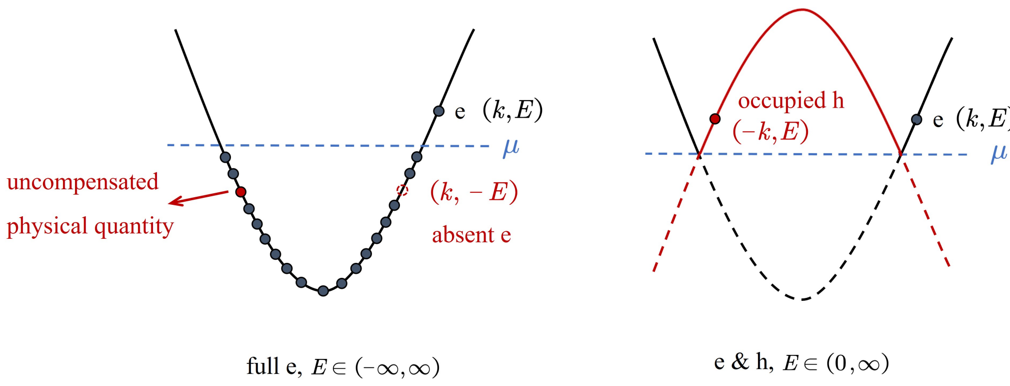
For the Bogoliubov quasi-particle operator, we have

$$\gamma_\sigma^\dagger(E) = \gamma_{\bar{\sigma}}(-E) \tag{3.82}$$

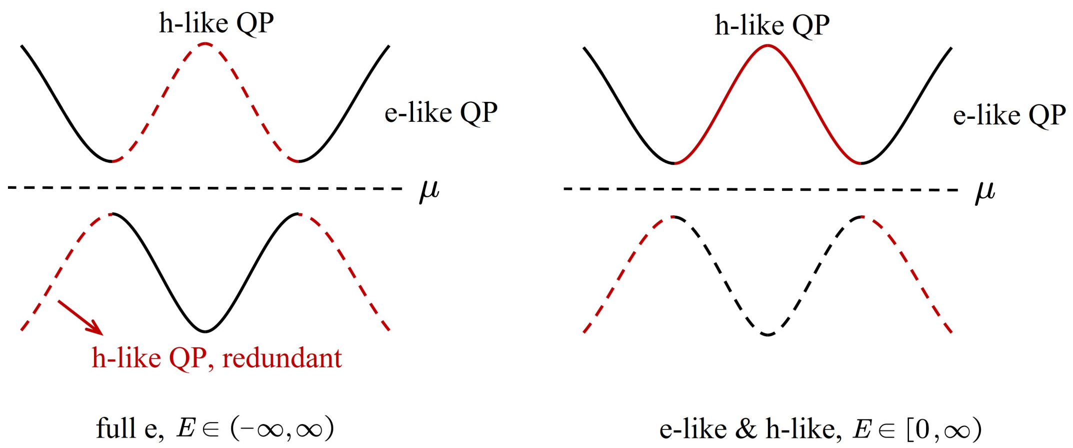
[6]The following derivation does not rely on representation.

meaning that creating a QP of energy E is equivalent to annihilating one with energy $-E$[7]. Therefore, we only need to focus on half of the degree of freedom. Take the trivial case as an example: normal metal (A trivial case but good benchmark)

1. full electron language: $H_N = \frac{p^2}{2m} - \mu$
2. BdG language: $H_{BdG} = \frac{1}{2}\begin{pmatrix} H_N & 0 \\ 0 & -H_N \end{pmatrix}$



To avoid the double counting in the BdG representation, we only focus on the part with positive energy. The same spirit is followed is the nontrivial case with finite pairing.



e-like: $\text{sgn}[v] = \text{sgn}[k]$; h-like: $\text{sgn}[v] = -\text{sgn}[k]$.

3.1.5 $e - h$ scattering (Andreev reflection), PH symmetry of S-matrix

Considering a normal metal-superconductor interface.

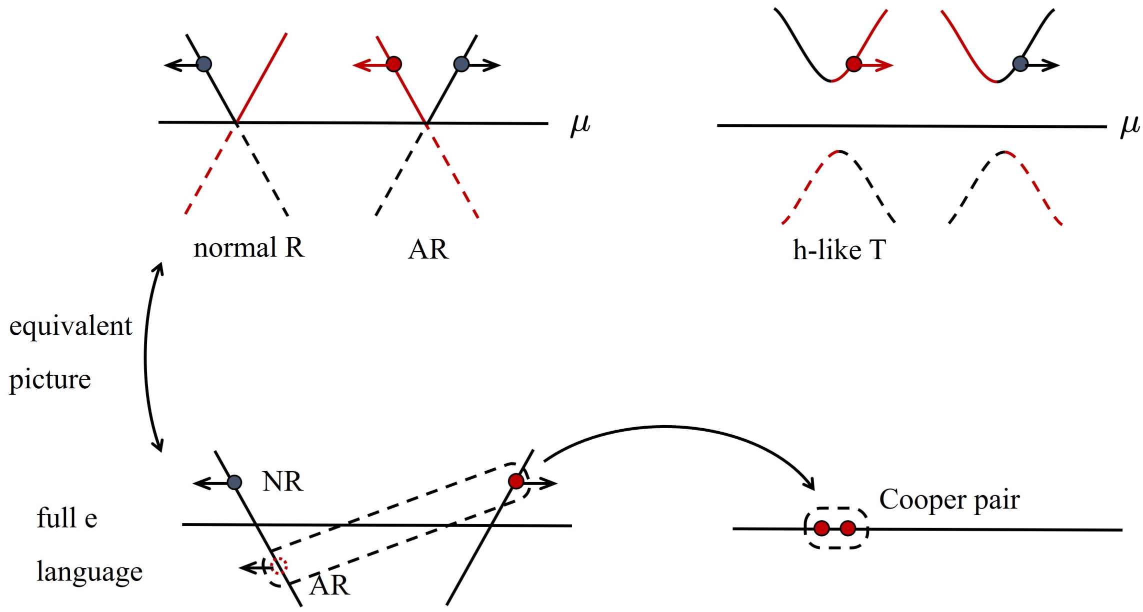
Question: $E \in [-\Delta, \Delta]$, *DOS*$= 0$ *for Superconductor, what happens?*

BdG equation:

$$i\hbar\partial_t \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} -\frac{\hbar^2\nabla^2}{2m} - \mu(x) + V(x) & \Delta(x) \\ \Delta^*(x) & \frac{\hbar^2\nabla^2}{2m} + \mu(x) - V(x) \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} \tag{3.83}$$

where $\Delta(x) = \theta(x)\Delta$ with Δ presumed to be a real quantity (disregard the unimportant $U(1)$ phase), and $V(x) = H\delta(x)$ is a Dirac-function-type barrier.

[7]Majorana, spinless quasi-particle at zero energy: $\gamma^\dagger(0) = \gamma(0)$, its *antiparticle* is identical to itself and can be utilized in *topological computing*. Topological ground state degeneracy. $e \equiv h$ + CP (unconserved).



plane-wave ansatz:

$$\begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix} e^{i(kx-Et/\hbar)} \tag{3.84}$$

For an eigenenergy E, the eigenstates are

1. electron-like:

$$\psi_{\pm k^+} = \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} e^{i\pm k^+ x} \tag{3.85}$$

2. hole-like

$$\psi_{\pm k^-} = \begin{pmatrix} v_0 \\ u_0 \end{pmatrix} e^{\pm i\pm k^- x} \tag{3.86}$$

$$u_0^2 = 1 - v_0^2 = \frac{1}{2}(1 + \sqrt{E^2 - \Delta^2}/E) \tag{3.87}$$

$$\hbar k^\pm = \sqrt{2m}\sqrt{\mu \pm (E^2 - \Delta^2)^{1/2}} \tag{3.88}$$

Δ is finite for superconductor, $\Delta = 0$ for normal metal.

Scattering state: For normal metal ($x < 0$):

$$\psi_N = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{iq^+ x} + a \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{iq^- x} + b \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-iq^+ x} \tag{3.89}$$

and for superconductor ($x > 0$):

$$\psi_S = c \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} e^{ik^- x} + d \begin{pmatrix} v_0 \\ u_0 \end{pmatrix} e^{-ik^+ x} \tag{3.90}$$

assuming $E_F \equiv \mu \gg \Delta$, it follows that $k^\pm \simeq q^\pm \simeq k_F$.

Boundary condition:

$$\begin{cases} \psi_S(0) = \psi_N(0) = \psi(0) & \text{continuity} \\ \psi_S'(0) - \psi_N'(0) = \frac{2mH}{\hbar^2}\psi(0) & \text{discontinuity} \end{cases} \tag{3.91}$$

then we can obtain the scattering coefficient.

Exercise 3.3 Prove the current conservation of quasi-particles in Andreev reflection problem:

$$\partial_t \rho + \nabla \cdot \vec{J}_\rho = 0$$

where $\rho = |f|^2 + |g|^2$, and $\vec{J}_\rho = \frac{\hbar}{m}\left[\mathrm{Im}(f^*\nabla f) - \mathrm{Im}(g^*\nabla g)\right]$.

Current conservation of QPs, rather than electrons

$$\partial\rho/\partial_t + \nabla \cdot \vec{J}_\rho = 0 \tag{3.92}$$

where $\rho = |f|^2 + |g|^2$, and $\vec{J}_\rho = \frac{\hbar}{m}\left[\mathrm{Im}(f^*\nabla f) - \mathrm{Im}(g^*\nabla g)\right]$.

Proof

$$i\hbar\partial_t \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} -\frac{\hbar^2\nabla^2}{2m} - \mu(x) + V(x) & \Delta(x) \\ \Delta^*(x) & \frac{\hbar^2\nabla^2}{2m} + \mu(x) - V(x) \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} \tag{3.93}$$

$$-i\hbar\partial_t \begin{pmatrix} f^* \\ g^* \end{pmatrix} = \begin{pmatrix} -\frac{\hbar^2\nabla^2}{2m} - \mu(x) + V(x) & \Delta(x) \\ \Delta^*(x) & \frac{\hbar^2\nabla^2}{2m} + \mu(x) - V(x) \end{pmatrix} \begin{pmatrix} f^* \\ g^* \end{pmatrix} \tag{3.94}$$

then $(f^*, g^*) \times$ (3.93) $- (f, g) \times$ (3.94):

$$\Rightarrow i\hbar\partial_t(ff^* + gg^*) = (f^*, g^*) \begin{pmatrix} -\frac{\hbar^2\nabla^2}{2m} - \mu(x) + V(x) & \Delta(x) \\ \Delta^*(x) & \frac{\hbar^2\nabla^2}{2m} + \mu(x) - V(x) \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} \tag{3.95}$$

$$- (f, g) \begin{pmatrix} -\frac{\hbar^2\nabla^2}{2m} - \mu(x) + V(x) & \Delta(x) \\ \Delta^*(x) & \frac{\hbar^2\nabla^2}{2m} + \mu(x) - V(x) \end{pmatrix} \begin{pmatrix} f^* \\ g^* \end{pmatrix} \tag{3.96}$$

$$= (f^*, g^*) \begin{pmatrix} (-\frac{\hbar^2\nabla^2}{2m} - \mu + V)f + \Delta g \\ \Delta f - (\frac{\hbar^2\nabla^2}{2m} + \mu - V)g \end{pmatrix} \tag{3.97}$$

$$= f^*(-\frac{\hbar^2\nabla^2}{2m} \cancel{- \mu + V})f + \cancel{f^*\Delta g} + \cancel{g^*\Delta f} + g^*(\frac{\hbar^2\nabla^2}{2m} + \cancel{\mu - V})g \tag{3.98}$$

$$- f(-\frac{\hbar^2\nabla^2}{2m} \cancel{- \mu + V})f^* - \cancel{f\Delta g^*} - \cancel{g\Delta f^*} - g(\frac{\hbar^2\nabla^2}{2m} + \cancel{\mu - V})g^* \tag{3.99}$$

$$= \frac{\hbar^2}{2m}[f\nabla^2 f^* - f^*\nabla^2 f - g\nabla^2 g^* + g^*\nabla^2 g] \tag{3.100}$$

$$= \frac{\hbar^2}{2m}\nabla \cdot [f\nabla f^* - f^*\nabla f - g\nabla g^* + g^*\nabla g] \tag{3.101}$$

$$\Rightarrow \partial_t(f^*f + g^*g) + i\frac{\hbar}{2m}\nabla \cdot [f\nabla f^* - f^*\nabla f - g\nabla g^* + g^*\nabla g] = 0 \tag{3.102}$$

$$\Rightarrow \partial_t\rho + \frac{\hbar}{2m}\nabla \cdot [-if^*\nabla f + if\nabla f^* - ig\nabla g^* + ig^*\nabla g] = 0 \tag{3.103}$$

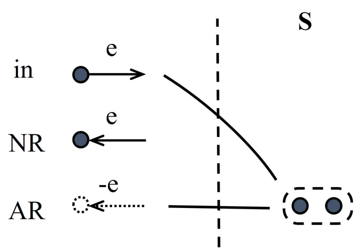
$$\Rightarrow \partial_t\rho + \frac{\hbar}{2m}\nabla \cdot [2\mathrm{Im}(f^*\nabla f) - 2\mathrm{Im}(g^*\nabla g)] = 0 \tag{3.104}$$

$$\Rightarrow \partial_t\rho + \nabla \cdot \frac{\hbar}{m}[\mathrm{Im}(f^*\nabla f) - \mathrm{Im}(g^*\nabla g)]^{8} = 0 \tag{3.105}$$

$$\Rightarrow \partial_t\rho + \nabla \cdot \vec{J}_\rho = 0 \tag{3.106}$$

In a scattering problem, the current conservation is an important criterion for checking the correctness of the calculation. Here, specifically we have

$$v_F \times 1 = v_F(A + B) + v_s(C + D) \tag{3.107}$$



[8] $\vec{J}_\rho = \frac{\hbar\vec{k}}{m}(|u|^2 - |v|^2) \propto \frac{\partial E}{\hbar\partial\vec{k}}$ is the velocity of QP.

For $E < \Delta$, $v_s = 0$, so that $A + B = 1$, indicating complete reflection.

Note that electron and hole possess opposite charge, so that the AR process contributes to charge transport.

3.1.5.1 PH symmetry of S-matrix

The particle-hole symmetry of the BdG Hamiltonian imposes constraint on the S-matrix, similar to the TR case. Without loss of generality, we use Φ_1 representation.

PH operation:

$$\Xi_1 \Psi_{\tau} = \Psi_{\bar{\tau}}^{*} \tag{3.108}$$

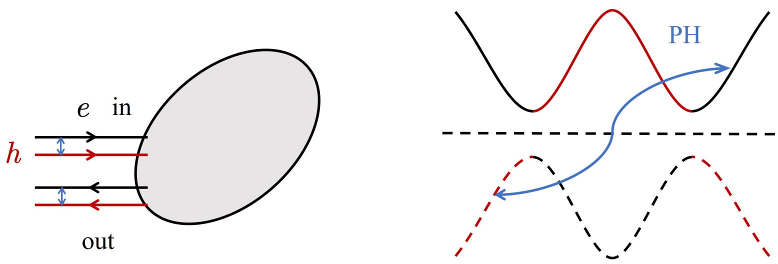
where τ_x: $e \leftrightarrow h$ exchange of $e - h$ component, anti-unitarity: Complex conjugation.

In the energy-momentum space (stationary states for scattering problem)

$$\Xi_1 \psi_{\tau}(E, k) = \psi_{\bar{\tau}}^{*}(-E, -k) \tag{3.109}$$

Note that PH operation does not change the group velocity of QP:

$$v_k = \frac{\partial E}{\hbar \partial_k} = \frac{\partial(-E)}{\hbar \partial(-k)} \tag{3.110}$$



PH-operation in typical incoming and outgoing states:

$$\Xi_1 \psi_{\tau}^{(in)}(E, k) = \psi_{\bar{\tau}}^{(in)}(-E, -k) \tag{3.111}$$

$$\Xi_1 \psi_{\tau}^{(out)}(E, k) = \psi_{\bar{\tau}}^{(out)}(-E, -k) \tag{3.112}$$

then consider the general incoming and outgoing states for a given energy:

$$\Psi^{(in)}(E) = \sum_{q\tau=e,h} a_{q\tau}(E) \psi_{q\tau}^{(in)}(E) \tag{3.113}$$

$$\Psi^{(out)}(E) = \sum_{p\tau'=e,h} b_{p\tau'}(E) \psi_{p\tau'}^{(out)}(E) \tag{3.114}$$

The coefficients are related by the S-matrix, or explicitly,

$$\{b\} = [S]\{a\} \iff \{b\}_{\tau'} = \sum_{\tau} [S]_{\tau'\tau} \{a\}_{\tau} \tag{3.115}$$

Perform PH transformation on the scattering states

$$\Psi^{(in)}_{new}(-E) = \Xi_1 \Psi^{(in)}(E) = \Xi_1 \sum_{q\tau} a_{q\tau}(E)\psi^{in}_{q\tau}(E) \tag{3.116}$$

$$= \sum_{q\tau} a^*_{q\tau}(E)\Xi_1\psi^{(in)}_{q\tau}(E) = \sum_{q\tau} a^*_{q\tau}(E)\psi^{(in)}_{q\bar{\tau}}(-E) \tag{3.117}$$

$$\Psi^{(out)}_{new}(-E) = \Xi_1 \Psi^{(out)}(E) = \Xi_1 \sum_{p\tau'} b_{p\tau'}(E)\psi^{in}_{p\tau'}(E) \tag{3.118}$$

$$= \sum_{p\tau'} b^*_{p\tau'}(E)\Xi_1\psi^{(out)}_{p\tau'}(E) = \sum_{p\tau'} b^*_{p\tau'}(E)\psi^{(out)}_{p\bar{\tau}'}(-E) \tag{3.119}$$

Similar to TR, the PH symmetry is reflected in two aspects:

(a). $\psi^{(in)}(E), \Xi_1\psi^{(in)}(E)$ are PH partners and establish the connection by comparing $\Psi^{(in)}(E)$, $\Psi^{(in)}_{new}(-E)$, $\Psi^{(out)}_{new}(-E)$ as follows:

$$a^*_{q\tau}(E) \leftrightarrow a_{q\bar{\tau}}(-E), \qquad b^*_{p\tau'} \leftrightarrow b_{p\bar{\tau}'}(-E) \tag{3.120}$$

(b). The states before and after the PH transformation satisfy the same BdG equation.

Rewrite the correspondence as

$$a_{q\tau}(E) \leftrightarrow a^*_{q\bar{\tau}}(-E), \qquad b^*_{q\tau'} \leftrightarrow b_{p\bar{\tau}'}(-E) \tag{3.121}$$

$$\Rightarrow \{b\}^*_{\bar{\tau}'}(-E) = \sum_{\tau}[S]_{\tau'\tau}(E)\{a\}^*_{\bar{\tau}}(-E) \tag{3.122}$$

$$(\bar{\tau} \to \tau, E \to -E) \qquad \Rightarrow \{b\}^*_{\tau'}(E) = \sum_{\tau}[S]^*_{\bar{\tau}'\bar{\tau}}(-E)\{a\}_{\tau}(E) \tag{3.123}$$

Comparing Eq. (3.115) and (3.123) yields

$$[S]_{\tau'\tau}(E) = [S]^*_{\bar{\tau}'\bar{\tau}}(-E) \tag{3.124}$$

This is the PH symmetry of the S-matrix, which is a strong restriction. For example, two types of AR processes are related as:

$$S_{eh}(E) = S^*_{he}(-E) \tag{3.125}$$

Two types of NR processes are related as:

$$S_{ee}(E) = S^*_{hh}(-E) \tag{3.126}$$

Like TR symmetry, the PH symmetry is a general symmetry. As long as the system can be described by the BdG Hamiltonian, then it holds.

3.1.5.2 BTK formula [9]

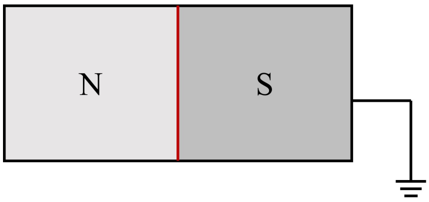
Assumption *Similar to the LB spirit, the incident particle (e or h) inherits the distribution of the electrons. The difference is that now the incident particle can be e or h.*

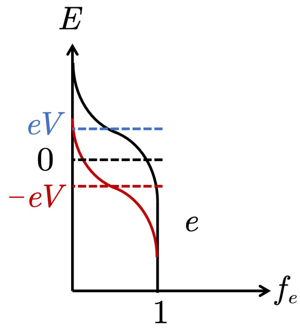
- Electron distribution:

$$f_e(E) = f(E - eV) \tag{3.127}$$

where V is the bias voltage.

[9]Reference: PRB: 25, 4515 (1982)





- Hole distribution:

$$f_h(E) = 1 - f_e(-E) = 1 - \frac{1}{1 + e^{(-E-eV)/k_BT}} \tag{3.128}$$

$$= \frac{e^{-(E+eV)}/k_BT}{1 + e^{-(E+eV)}/k_BT} \tag{3.129}$$

$$= \frac{1}{e^{-(E+eV)}/k_BT} = f(E+eV) \tag{3.130}$$

Note *The current can be calculated at any cross section. Since the electron number is not conserved in Superconductor, it is convenient to calculate the current in Normal metal.*

$$I = 2N(0)ev_F\mathcal{A}\int_0^\infty dE\,\{[f(E-eV) - f(E)][1 + A(E) - B(E)] + [f(E+eV) - f(E)][(-1 - A^h(E) + B^h(E))]\} \tag{3.131}$$

$N(0)$ is the DOS in normal metal (without spin) and $\mathcal{A}$ is the cross-section area. The integral for $E > 0$ in the aforementioned equation is designed to prevent redundancy. Here, $A(E)$ denotes the AR reflection, and minus sign in the red term due to the hole's opposite charge.

In normal metal, the number of conducting electrons *per unit energy* is

$$2N(0)V_0 \tag{3.132}$$

where V_0 is the volume of normal metal. Thus, current is

$$2ev_FN(0)V_0/L = 2ev_FN(0)\mathcal{A} \tag{3.133}$$

where L is the length of normal metal.

The total current is:

$$I = 2N(0)ev_F\mathcal{A}\int_0^\infty dE\,\{[f(E-eV) - f(E)][1 + A(E) - B(E)] + [f(E+eV) - f(E)][-1 - A^h(E) + B^h(E)]\} \tag{3.134}$$

$$= 2N(0)ev_F\mathcal{A}\left\{\int_0^\infty dE[f(E-eV) - f(E)][1 + A(E) - B(E)] + \int_{-\infty}^0 [f(-E+eV) - f(-E)][-1 - A^h(-E) + B^h(-E)]\right\} \tag{3.135}$$

Considering PH symmetry:

$$A^h(-E) = A(E), \qquad B^h(-E) = B(E) \tag{3.136}$$

$$f(-E) = \frac{1}{e^{-E/k_BT}} = 1 - \frac{1}{1 + e^{E/k_BT}} = 1 - f(E) \tag{3.137}$$

then we obtain:

$$I = 2N(0)ev_F\mathcal{A}\left\{\int_0^{\infty} dE[f(E-eV)-f(E)][1+A(E)-B(E)]\right.$$
$$\left.+\int_{-\infty}^{0}[f(E)-f(E-eV)](-1)[1+A^h(E)-B^h(E)]\right\} \tag{3.138}$$
$$\Rightarrow I = 2N(0)ev_F\mathcal{A}\int_{-\infty}^{\infty} dE\,[f(E-eV)-f(E)][1+A(E)-B(E)] \tag{3.139}$$

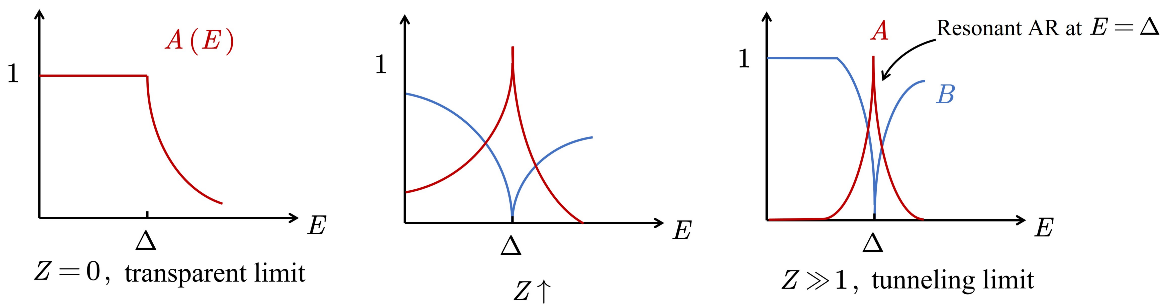
where the last equation is BTK formula[10]. At temperatures satisfying $T \ll \Delta$, where $f(E) \simeq \theta(E)$, this equation can be simplified:

$$\Rightarrow I = 2N(0)ev_F\mathcal{A}\int_0^{eV} dE[1+A(E)-B(E)] \tag{3.140}$$
$$\Rightarrow G = \frac{\partial I}{\partial V} \propto 1 + A(eV) - B(eV) \tag{3.141}$$

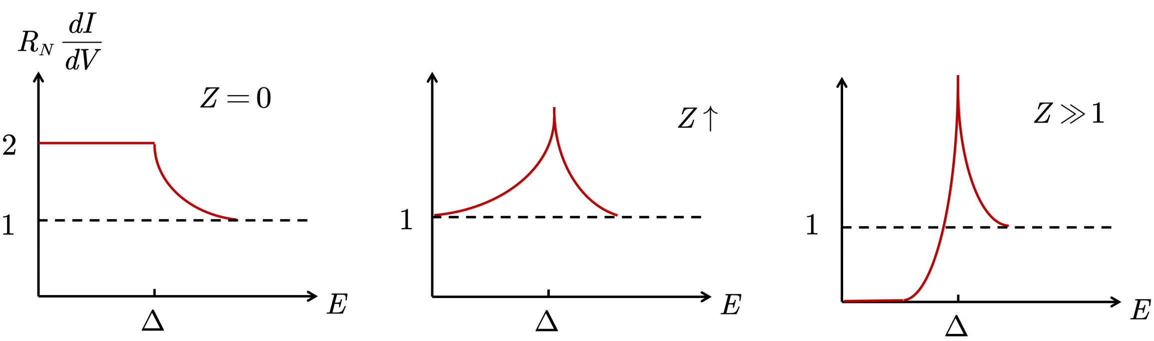
where $G = \partial I/\partial V$ is the differential conductance.

Remark In the $\Delta = 0$ limit, superconductor reduces to normal metal. The $A(E) = 0$, $1 - B(E) = T(E)$ transmission, reduces to the LB formula. Therefore, BTK formula is the extension of LB formula to the Nambu space.

- **Typical features of the scattering probabilities**[11]**:**



- **Differential conductance:**



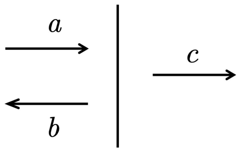
3.1.5.3 Simple examples, junction

Herbert Kroemer: "*The interface is the device.*"

[10] Reference: [PRB 25, 4515 (1982), Milestone]

[11] In-gap, $\Delta < 0$, $A + B = 1$.

General steps for these problem:

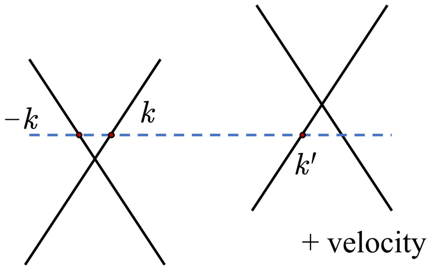


- Step 1:

$$\text{Hamiltonian} \rightarrow \begin{cases} \text{Current conservation} \\ \text{Boundary condition (BC)} \end{cases} \qquad \text{(consistency)} \tag{3.142}$$

- Step 2: Solving scattering states, coefficient using boundary condition. (check current conservation)

Example 3.1 Klein tunneling for Dirac fermion (Graphene, Topological surface state):



The Hamiltonian for 1D Dirac fermion:

$$H = \sigma_x k + V \tag{3.143}$$

where $V = V_0\theta(x)$.

Eigenvalue equation:

$$H\psi(x) = E\psi(x) \tag{3.144}$$

$$\Rightarrow \begin{cases} \psi_L(x) = e^{ikx}\begin{pmatrix}1\\1\end{pmatrix} + be^{-ikx}\begin{pmatrix}-1\\1\end{pmatrix} & k = E \\ \psi_R(x) = ce^{ik'x}\begin{pmatrix}1\\1\end{pmatrix} & k' = E - V_0 \end{cases} \tag{3.145}$$

(speudo-)spin momentum locking.

Boundary condition:

$$\psi_L(0) = \psi_R(0) \Rightarrow c = 1 \tag{3.146}$$

$$J = \psi^\dagger \sigma_x \psi \Rightarrow |c|^2 = 1 \tag{3.147}$$

This implies that the incoming current is equivalent to the outgoing current, thereby satisfying the principle of current conservation.

Reflection: $|b|^2 = 0$, indicating no reflection.

- key-point: Spin-momentum locking.
- Another point is scattering problems, the match of velocities on both sides.

For systems with irregular shapes, the solution need numerics.

Example 3.2 $\delta(x)$ barrier:

Eigenvalue equation:

$$\left[-\frac{\hbar^2}{2m}\partial_x^2 + U\delta(x)\right]\psi(x) = E\psi(x) \tag{3.148}$$

To obtain the boundary condition, integral from 0^- to 0^+

$$-\frac{\hbar^2}{2m}\int_{0^-}^{0^+}\psi'' + U\int_{0^-}^{0^+}\delta(x)\psi(x) = \int_{0^-}^{0^+}E\psi(x) = 0 \tag{3.149}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left[\psi'(0^+) - \psi'(0^-)\right] + U\psi(0) = 0 \tag{3.150}$$

$$\Rightarrow \begin{cases}\psi'(0^+) - \psi'(0^-) = \frac{2mU}{\hbar^2}\psi(0)\\ \psi(0^+) = \psi(0^-) = \psi(0)\end{cases} \tag{3.151}$$

Check current conservation $J(0^-) = J(0^+)$:

$$J(x) = \frac{\hbar}{2mi}\left[\psi^*(x)\partial_x\psi(x) - \partial_x\psi^*(x)\psi(x)\right] \tag{3.152}$$

$$J(0^+) = \frac{\hbar}{2mi}\left[\psi^*(0^+)\psi'(0^+) - \psi'^*(0^+)\psi(0^+)\right] \tag{3.153}$$

$$= \frac{\hbar}{2mi}\left\{\psi^*(0)\left[\cancel{\frac{2mU}{\hbar^2}\psi(0)} + \psi'(0^-)\right] - \left[\cancel{\frac{2mU}{\hbar^2}\psi^*(0)} + \psi^{*\prime}(0^-)\right]\psi(0)\right\} \tag{3.154}$$

$$= \frac{\hbar}{2mi}\left[\psi^*(0^-)\psi'(0^-) - \psi^{*\prime}(0^-)\psi(0^-)\right] = J(0^-) \tag{3.155}$$

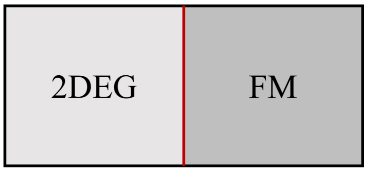
Example 3.3 Hetero-Junction:

Hamiltonian:

$$\begin{cases}H_R = \frac{p^2}{2m_R} + \alpha_R(k_x\sigma_y - k_y\sigma_x) - \mu_R\\ H_F = \frac{p^2}{2m_F} + M_z\sigma_z - \mu_F\end{cases} \tag{3.156}$$

we replace: $k_x \to -i\partial_x$, $k_y \to$number:

$$H = H_R\theta(-x) + H_F\theta(x) \tag{3.157}$$



Non-Hermitian! Broken current conservation.

To address the issue, we need to make the Hamiltonian symmetric/Hermitian. (The way is not unique).

$$m(x) = m_R\theta(-x) + m_F\theta(x) \tag{3.158}$$

$$\alpha_R(x) = \alpha_R\theta(-x) \tag{3.159}$$

Other terms are $\theta(\pm x)\times$ const. Doesn't matter.

Kinetic energy:

$$\left[-\frac{\hbar^2}{2m(x)\partial_x^2}\right]^\dagger = -\partial_x^2\frac{\hbar^2}{2m(x)} \neq h_k \tag{3.160}$$

$$\text{(modify)}\qquad \Rightarrow -\frac{\hbar^2}{2}\partial_x\frac{1}{m(x)}\partial_x \tag{3.161}$$

Rashba SOC:

$$\left[-i\alpha_R\theta(-x)\partial_x\sigma_y\right]^\dagger = -i\alpha_R\partial_x\theta(-x)\sigma_y \neq h_R \tag{3.162}$$

$$\text{(modify)}\qquad \Rightarrow -\frac{i}{2}\{\alpha_R(x),\partial_x\}\sigma_y \tag{3.163}$$

modified H:

$$\tilde{H} = -\hbar^2\partial_x\frac{1}{2m(x)}\partial_x - \frac{i}{2}\{\alpha_R(x),\partial_x\}\sigma_y + c_1\theta(x) + c_2\theta(-x) \tag{3.164}$$

The red terms are not important for boundary condition.

Eigenvalue equation:

$$\tilde{H}(x)\psi(x) = E\psi(x) \tag{3.165}$$

$$\Rightarrow \int_{0^-}^{0^+} \tilde{H}(x)\psi(x)dx = 0 \tag{3.166}$$

$$\Rightarrow -\hbar^2 \int_{0^-}^{0^+} \partial_x \frac{1}{2m(x)} \partial_x \psi(x)dx - \frac{i}{2}\sigma_y \int_{0^-}^{0^+} \{\alpha_R(x), \partial_x\}\psi(x)dx = 0 \tag{3.167}$$

$$\Rightarrow -\hbar^2 \frac{1}{2m(x)}\psi'(x)|_{0^-}^{0^+} - \frac{i}{2}\sigma_y\alpha_R \int_{0^-}^{0^+} \{\theta(-x), \partial_x\}\psi(x)dx = 0 \tag{3.168}$$

$$\Rightarrow \hbar^2 \frac{1}{m(0^-)}\psi'(0^-) - \hbar^2 \frac{1}{m(0^+)}\psi'(0^+) = i\sigma_y\alpha_R \int_{0^-}^{0^+} \left[\theta(-x)\psi'(x) + \partial_x \left(\theta(x)\psi(x)\right)\right] dx \tag{3.169}$$

$$= i\sigma_y\alpha_R\theta(-x)\psi(x)|_{0^-}^{0^+} = -\frac{i}{2}\sigma_y\alpha_R\psi(0) \tag{3.170}$$

$$\Rightarrow \frac{1}{m(0^+)}\psi'(0^+) - \frac{1}{m(0^-)}\psi'(0^-) = \frac{i}{\hbar^2}\sigma_y\alpha_R\psi(0) \tag{3.171}$$

So, the boundary condition:

$$\begin{cases} \frac{1}{m_F}\psi_F'(0) - \frac{1}{m_R}\psi_R'(0) = \frac{i}{2\hbar^2}\sigma_y\alpha_R\psi(0) \\ \psi_F(0) = \psi_R(0) = \psi(0) \end{cases} \tag{3.172}$$

Current:

$$J_R = \frac{\hbar}{2mi}\left[\psi^\dagger\partial_x\psi - (\partial_x\psi^\dagger)\psi\right] + \frac{\alpha_R}{\hbar}\psi^\dagger\sigma_y\psi \tag{3.173}$$

$$J_F = \frac{\hbar}{2m_F i}\left[\psi^\dagger\partial_x\psi - (\partial_x\psi^\dagger)\psi\right] \tag{3.174}$$

Current conservation:

$$J_R = J(0^-) = \frac{\hbar}{2m_R i}\left[\psi_R^\dagger(0)\psi_R'(0) - \psi_R^{\dagger\prime}(0)\psi_R(0)\right] + \frac{\alpha_R}{\hbar}\psi_R^\dagger\sigma_y\psi_R \tag{3.175}$$

$$= \frac{\hbar}{2m_R i}\left[\psi_F^\dagger(0)\psi_R'(0) - \psi_R^{\dagger\prime}(0)\psi_F(0)\right] + \frac{\alpha_R}{\hbar}\psi_R^\dagger\sigma_y\psi_R \tag{3.176}$$

$$= \frac{\hbar}{2i}\psi_F^\dagger(0)\left[\frac{1}{m_F}\psi_F'(0) - \frac{i}{\hbar^2}\sigma_y\alpha_R\psi(0)\right] - \frac{\hbar}{2i}\left[\frac{1}{m_F}\psi_F^{\dagger\prime}(0) + \frac{i}{\hbar^2}\alpha_R\psi^\dagger(0)\sigma_y\right]\psi_F(0) + \frac{\alpha_R}{\hbar}\psi_R^\dagger\sigma_y\psi_R \tag{3.177}$$

$$= \frac{\hbar}{2m_F i}\left[\psi_F^\dagger(0)\psi_F'(0) - \psi_F^{\dagger\prime}(0)\psi_F(0)\right] - \frac{\alpha_R}{\hbar}\psi_R^\dagger\sigma_y\psi_R + \frac{\alpha_R}{\hbar}\psi_R^\dagger\sigma_y\psi_R \tag{3.178}$$

$$= J_F \tag{3.179}$$

3.2 Combining S-matrices

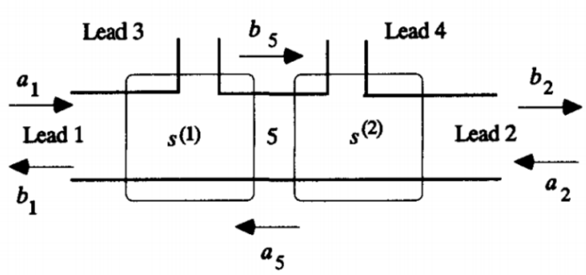
The S-matrices in different parts of the system can be combined with coherence.

$S = S_1 \otimes S_2$,

$$\begin{pmatrix} b_{13} \\ b_5 \end{pmatrix} = \begin{pmatrix} r_1 & t_1' \\ t_1 & r_1' \end{pmatrix}\begin{pmatrix} a_{13} \\ a_5 \end{pmatrix}, \quad \begin{pmatrix} a_5 \\ b_{24} \end{pmatrix} = \begin{pmatrix} r_2 & t_2' \\ t_2 & r_2' \end{pmatrix}\begin{pmatrix} b_5 \\ a_{24} \end{pmatrix} \tag{3.180}$$

where "t" are the transmission matrices, "r" are the reflection matrices,

$$(a_{13}) = \begin{pmatrix} \{a_1\} \\ \{a_3\} \end{pmatrix}, \quad (b_{13}) = \begin{pmatrix} \{b_1\} \\ \{b_3\} \end{pmatrix} \tag{3.181}$$



Eliminating a_5, b_5 to obtain the entire S-matrix,

$$\begin{cases} b_{13} = r_1 a_{13} + t_1' a_5 \\ b_5 = t_1 a_{13} + r_1' a_5 \end{cases} \qquad \begin{cases} a_5 = r_2 b_5 + t_2' a_{24} \\ b_{24} = t_2 b_5 + r_2' a_{24} \end{cases}$$

$$b_5 = t_1 a_{13} + r_1' r_2 b_5 + r_1' t_2' a_{24} \Rightarrow b_5 = (1 - r_1' r_2)^{-1}(t_1 a_{13} + r_1' t_2' a_{24}) \tag{3.182}$$

$$b_{24} = t_2(1 - r_1' r_2)^{-1}(t_1 a_{13} + r_1' t_2' a_{24}) + r_2' a_{24} = t_2(1 - r_1' r_2)^{-1} t_1 a_{13} + [t_2(1 - r_1' r_2)^{-1} r_1' t_2' + r_2'] a_{24} \tag{3.183}$$

$$a_5 = r_2(t_1 a_{13} + r_1' a_5) + t_2' a_{24} \Rightarrow a_5 = (1 - r_2 r_1')^{-1}(r_2 t_1 a_{13} + t_2' a_{24}) \tag{3.184}$$

$$b_{13} = r_1 a_{13} + t_1'(1 - r_2 r_1')^{-1}(r_2 t_1 a_{13} + t_2' a_{24}) = [r_1 + t_1'(1 - r_2 r_1')^{-1} r_2 t_1] a_{13} + t_1'(1 - r_2 r_1')^{-1} t_2' a_{24} \tag{3.185}$$

$$\begin{pmatrix} b_{13} \\ b_{24} \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} a_{13} \\ a_{24} \end{pmatrix} \tag{3.186}$$

where

$$\begin{cases} r = r = r_1 + t_1'(1 - r_2 r_1')^{-1} r_2 t_1 = r_1 + t_1' r_2 [1 + r_2 r_1' + (r_2 r_1')^2 + ...] r_2 t_1 \\ \quad = r_1 + t_1'[1 + r_2 r_1' + (r_2 r_1')^2 + ...] t_1 = r_1 + t_1' r_2 (1 - r_2 r_1')^{-1} t_1 \\ t' = t_1'(1 - r_2 r_1')^{-1} t_2' \\ t = t_2'(1 - r_1' r_2)^{-1} t_1' \\ r' = r_2' + t_2 (1 - r_1' r_2)^{-1} r_1' t_2' \end{cases}$$

Application: (a) Divide the whole system to several parts to ensure the computational capability. (b) Many phenomena can be described by the S-matrix in general forms, where only the basic properties such as unitarity, symmetry should be satisfied. The combination of S-matrix then can be useful in describing many effects.

3.2.1 Feynman paths

Insight form expanding the transmission matrix:

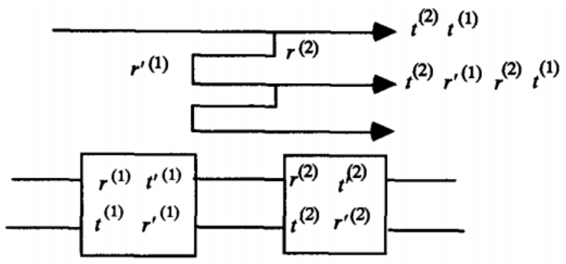
$$t = t_2(1 - r_1' r_2)^{-1} t_1 = t_2[1 + r_1' r_2 + (r_1' r_2)^2 + ...] t_1 \tag{3.187}$$

Specifically, for the matrix element (m,n), $t_{mn} = \sum_p A_p$, $p \in$ all path starting in mode n and ending in mode m. For example, the second term:

$$[t_2 r_1' r_2 t_1]_{mn} = \sum_{m_1} \sum_{m_2} \sum_{m_3} (t_2)_{mm_1} (r_1')_{m_1 m_2} (r_2)_{m_2 m_3} (t_1)_{m_3 n} \tag{3.188}$$

Transmission probability: $T_{mn} = |t_{m,n}|^2 = \sum_p A_p^* A_p + \sum_p \sum_{p' \neq p} A_p^* A_{p'}$.

For $L \gg l_\phi$, the second (interference) term $\simeq$0. Compare the simplest case with two sections, coherent:



amplitude $t = \frac{t_1 t_2}{1-r_1' r_2}$, probability

$$T = |t|^2 = \frac{T_1 T_2}{1 - 2\sqrt{R_1 R_2}\cos\theta + R_1 R_2} \tag{3.189}$$

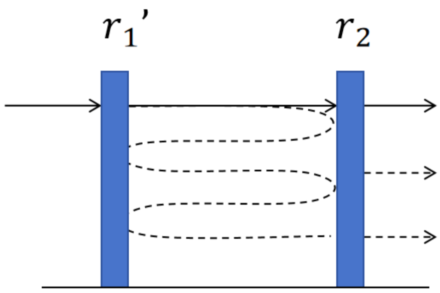
Incoherent: probability

$$T = \frac{T_1 T_2}{1 - \sqrt{R_1 R_2}} \tag{3.190}$$

where $T_{1,2} = |t_{1,2}|^2, R_{1,2} = |r_{1,2}'|^2, \theta = \text{Arg}(r_1') + \text{Arg}(r_2)$.

Remark Feynman paths provide a very useful perspective for understanding physical results rather than a computational tool.

Applications: Understanding resonance $\Leftrightarrow$ Bound states.



(i) Resonance tunneling, $t = t_2(1 - r_1' r_2)^{-1} t_1$. Resonance condition: $1 - r_1' r_2 = 0$. $\text{Arg}(r_1') \simeq e^{ik\cdot L}$, $\text{Arg}(r_2) \simeq e^{ik\cdot L}$, resonance occurs for weak tunneling $\Rightarrow e^{2ik\cdot L} = 1$, $2k \cdot L = 2n\pi$. The condition is exacting the same as that of forming bound states. Therefore, we can say that the resonance is induced by the bound state. More detail: $T = \frac{T_1 T_2}{1-2\sqrt{R_1 R_2}\cos\theta + R_1 R_2}$, $R_{1,2} = 1 - T_{1,2}$. Weak tunneling limit: $T_{1,2} \ll 1, R_1 R_2 \simeq 1 - T_1 - T_2$,

$$\begin{aligned} T = \frac{T_1 T_2}{(1-\sqrt{R_1 R_2})^2 + 2\sqrt{R_1 R_2}(1-\cos\theta)} &\simeq \frac{T_1 T_2}{[1-\sqrt{1-T_1-T_2}]^2 + 2\sqrt{1-T_1-T_2}(1-\cos\theta)} \\ &\simeq \frac{T_1 T_2}{[(T_1+T_2)/2]^2 + 2(1-\cos\theta)} \end{aligned} \tag{3.191}$$

Resonance level: $\cos[\theta(E_\mu)] = 1, \theta(E_\mu) = 2n\pi$. Near the level $E \sim E_\mu$,

$$\begin{aligned} \theta(E) \simeq \theta(E_\mu) + \delta\theta = 2n\pi + \frac{d\theta}{dE}\bigg|_{E_\mu}(E - E_\mu) \\ 1 - \cos\theta = 1 - \cos[2n\pi + \delta\theta] = 1 - \cos\delta\theta \simeq \frac{1}{2}\delta\theta^2 = \frac{1}{2}(\frac{d\theta}{dE}|_{E_\mu})^2(E - E_\mu)^2 \\ \Rightarrow T \simeq \frac{T_1 T_2}{[(T_1+T_2)/2]^2 + (\frac{d\theta}{dE}|_{E_\mu})^2(E-E_\mu)^2} \end{aligned} \tag{3.192}$$

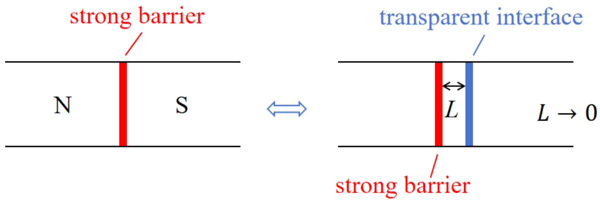
Define $\Gamma_{1,2} = T_{1,2}\frac{dE}{d\theta}\big|_{E_\mu}$,

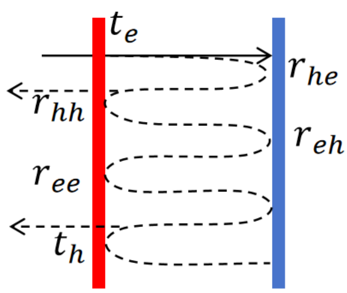
$$T \simeq \frac{\Gamma_1\Gamma_2}{[(\Gamma_1+\Gamma_2)/2]^2 + (E-E_\mu)^2} = \frac{\Gamma_1\Gamma_2}{\Gamma_1+\Gamma_2}\frac{\Gamma}{(\Gamma/2)^2+(E-E_\mu)^2} \tag{3.193}$$

where $\Gamma = \Gamma_1 + \Gamma_2$. Note that $\frac{\Gamma}{(\Gamma/2)^2+(E-E_\mu)^2}$ is a Lorentzian function. The resonance condition: $\Gamma_1 = \Gamma_2 \Rightarrow T = 1$ at $E = E_\mu$, equal coupling.

(ii) Majorana zero mode induced resonant Andreev reflection (AR)

Recall the resonant AR at $E = \Delta$ for conventional superconductor (s-wave). It can be analyzed as follows. Transparent N/S interface: AR amplitude for $E \leq \Delta$: $r_{he} = r_{eh} = e^{-i\cos^{-1}(E/\Delta)}$



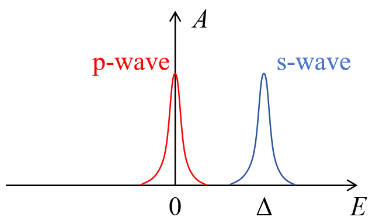


$$\tilde{r}_{he} = t_h(1 + r_{he}r_{ee}r_{eh}r_{hh} + ...)r_{he}t_e = \frac{t_h r_{he} t_e}{1 - r_{he}r_{ee}r_{eh}r_{hh}} \tag{3.194}$$

$r_{hh}(E) = r^*_{ee}(-E) \simeq r^*_{ee}(0) = r^*$, $\tilde{r}_{he} = \frac{t_h r_{he} t_e}{1 - R r_{he} r_{eh}} = \frac{t_h r_{he} t_e}{1 - R r^2_{he}(E)}$.

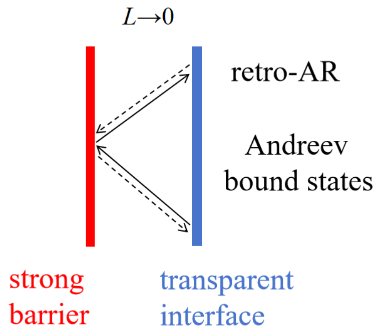
Remark Here, $r_{eh}(E) \neq r^*_{he}(-E) = -r_{eh}(E)$, but it does not break the particle-hole (PH) symmetry. In particular, PH symmetry should involve a spin inversion as well. We have $r^\sigma_{eh}(E) = r^{\bar{\sigma}*}_{he}(-E) = -r^{\sigma*}_{he}(-E) = r^\sigma_{eh}(E)$. For opposite spin, $\Delta \to -\Delta$. This minus sigh is inherited by the AR amplitude.

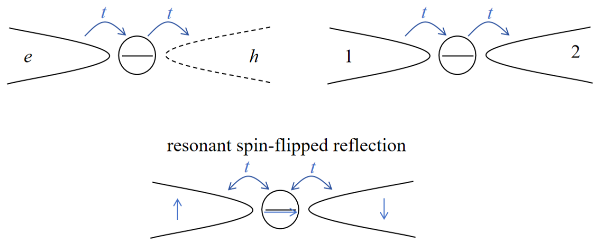
Resonance condition: $1 - R r^2_{he}(E) = 0, R \sim 1, 1 - e^{-2i\cos^{-1}(E/\Delta)} = 0, \Rightarrow 2\cos^{-1}(E/\Delta) = 0 \Rightarrow E = \Delta$. For 1D p-wave (Kitaev chain), $\Delta(k) = -\Delta(-k) \propto k$. PH operation: involve $\Delta \to -\Delta, \Rightarrow r_{eh} = -r_{he} = e^{i\pi}r_{he} \Rightarrow 1 + e^{-2i\cos^{-1}(E/\Delta)} = 0 \Rightarrow 2\cos^{-1}(E/\Delta) = \pi \Rightarrow E = 0 \Rightarrow$ zero-bias conductance peak (ZBCP).



$E = 0$, in gap $\Rightarrow$ band state: Majorana bound state. Recent experiment progress remains controversial. ZBCP is not the smoking gun evidence.

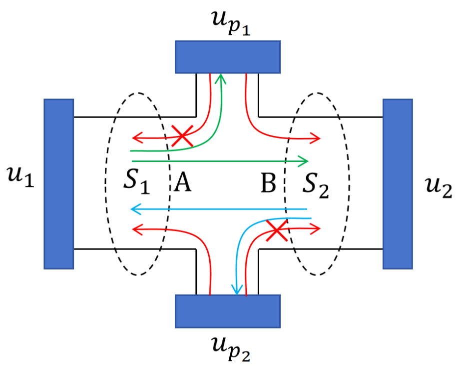
relation between resonant AR and resonant tunneling:





3.2.2 Partial coherence, virtual voltage probe

We only want to introduce decoherence effect. However, the additional probe may introduce unwanted momentum relaxation. Solution: unidirectional probes.



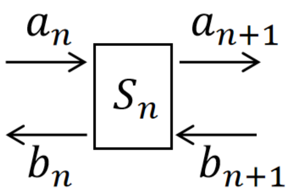
$A \Rightarrow B$ ($\sqrt{1-\alpha}$) or p_1 ($\sqrt{\alpha}$), $p_1 \Rightarrow B$ ($-\sqrt{\alpha}$), $B \Rightarrow A$ ($\sqrt{1-\alpha}$) or p_2 ($\sqrt{\alpha}$), $p_2 \Rightarrow A$ ($-\sqrt{\alpha}$). The S-matrix:

t_{nm}	A	B	p_1	p_2
A	0	$\sqrt{1-\alpha}$	0	$-\sqrt{\alpha}$
B	$\sqrt{1-\alpha}$	0	$-\sqrt{\alpha}$	0
p_1	$\sqrt{\alpha}$	0	$\sqrt{1-\alpha}$	0
p_2	0	$\sqrt{\alpha}$	0	$\sqrt{1-\alpha}$

(3.195)

$\alpha \in [0,1]$. In this four-terminal device, the Büttiker formula is in the linear response regime. $S_1 : 1, A$, $S_2 : 2, B$, $S : A, B, p_1, p_2$. Eliminate internal terminals $A, B \Rightarrow$ find $\widetilde{S}$-matrix: 1, 2, p_1, p_2. $(b_1, b_2, b_{p_1}, b_{p_2})^T = \widetilde{S}(a_1, a_2, a_{p_1}, b_{p_2}) \Rightarrow T_{pq} = |S_{pq}|^2, G_{pq} = \frac{2e}{h} T_{pq} \Rightarrow I_p = \sum_q G_{pq}[V_p - V_q]$. Condition: $I_{p_1} = I_{p_2} = 0$.

3.2.3 Transfer matrix method and relation with S-matrix



$$\begin{pmatrix} b_n \\ a_{n+1} \end{pmatrix} = [S_n] \begin{pmatrix} a_n \\ b_{n+1} \end{pmatrix} \Rightarrow \begin{pmatrix} a_n \\ b_n \end{pmatrix} = [M_n] \begin{pmatrix} a_{n+1} \\ b_{n+1} \end{pmatrix} \tag{3.196}$$

where M_n is the transfer matrix. The advantage of transfer matrix: A series of scatterers,

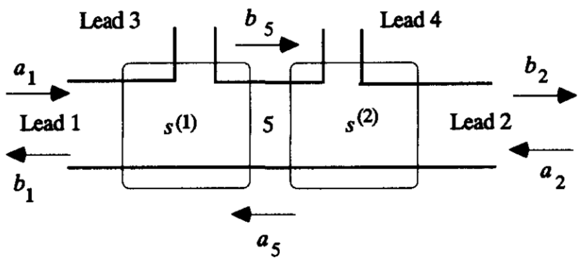
$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = [M_1] \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = [M_1 M_2] \begin{pmatrix} a_3 \\ b_3 \end{pmatrix} ... = [M_1 M_2 ... M_{N-1}] \begin{pmatrix} a_N \\ b_N \end{pmatrix} \tag{3.197}$$

✍ **Exercise 3.4** Considering a four-terminal Hall bridge as shown in Fig. We write the individual S-matrices in the form:

$$\begin{pmatrix} b_{13} \\ b_5 \end{pmatrix} = \begin{pmatrix} r_1 & t_1' \\ t_1 & r_1' \end{pmatrix} \begin{pmatrix} a_{13} \\ a_5 \end{pmatrix} \quad \begin{pmatrix} a_5 \\ b_{24} \end{pmatrix} = \begin{pmatrix} r_2 & t_2' \\ t_2 & r_2' \end{pmatrix} \begin{pmatrix} b_5 \\ a_{24} \end{pmatrix}$$

Now, try to eliminate a_5 and b_5 from the above equations to obtain the S-matrix $S = S_1 \otimes S_2 = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}$ for the composite structure:

$$\begin{pmatrix} b_{13} \\ b_{24} \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} a_{13} \\ a_{24} \end{pmatrix}$$



Solution *Eliminating a_5, b_5 to obtain the entire S-matrix,*

$$\begin{cases} b_{13} = r_1 a_{13} + t_1' a_5 \\ b_5 = t_1 a_{13} + r_1' a_5 \end{cases} \qquad \begin{cases} a_5 = r_2 b_5 + t_2' a_{24} \\ b_{24} = t_2 b_5 + r_2' a_{24} \end{cases}$$

$$b_5 = t_1 a_{13} + r_1' r_2 b_5 + r_1' t_2' a_{24} \Rightarrow b_5 = (1 - r_1' r_2)^{-1} (t_1 a_{13} + r_1' t_2' a_{24})$$

$$b_{24} = t_2 (1 - r_1' r_2)^{-1} (t_1 a_{13} + r_1' t_2' a_{24}) + r_2' a_{24} = t_2 (1 - r_1' r_2)^{-1} t_1 a_{13} + [t_2 (1 - r_1' r_2)^{-1} r_1' t_2' + r_2'] a_{24}$$

$$a_5 = r_2 (t_1 a_{13} + r_1' a_5) + t_2' a_{24} \Rightarrow a_5 = (1 - r_2 r_1')^{-1} (r_2 t_1 a_{13} + t_2' a_{24})$$

$$b_{13} = r_1 a_{13} + t_1' (1 - r_2 r_1')^{-1} (r_2 t_1 a_{13} + t_2' a_{24}) = [r_1 + t_1' (1 - r_2 r_1')^{-1} r_2 t_1] a_{13} + t_1' (1 - r_2 r_1')^{-1} t_2' a_{24}$$

one obtains

$$\begin{pmatrix} b_{13} \\ b_{24} \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} a_{13} \\ a_{24} \end{pmatrix}$$

where

$$\begin{cases} r = r_1 + t_1'(1 - r_2 r_1')^{-1} r_2 t_1 \\ t' = t_1'(1 - r_2 r_1')^{-1} t_2' \\ t = t_2'(1 - r_1' r_2)^{-1} t_1' \\ r' = r_2' + t_2(1 - r_1' r_2)^{-1} r_1' t_2' \end{cases}$$

✍ **Exercise 3.5** *Majorana zero mode induced resonant Andreev Reflection.* Considering a N/S interface as shown in Fig, where a strong barrier is present at the interface. The Andreev reflection amplitude for an s-wave superconductor at a transparent N/S interface with $E \leq \Delta$ is given by:

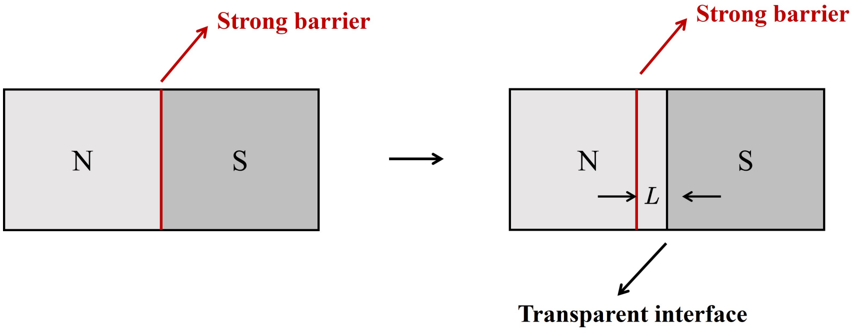
$$r_{eh} = r_{he} = e^{-i\cos^{-1}(\frac{E}{\Delta})}, \tag{3.198}$$

and for a p-wave superconductor, the reflection amplitude is given by:

$$r_{eh} = e^{i\pi} r_{he} = -e^{-i\cos^{-1}(\frac{E}{\Delta})}. \tag{3.199}$$

Determine the resonant energy in both the s-wave and p-wave cases.

Hint: We can place the strong barrier in the normal metal at a distance L from the interface, and then take the limit as $L \to 0$.



Solution *Taking into account the resonance scattering depicted in Fig.E.4, the resonant tunneling amplitude can be articulated as:*

$$\tilde{r}_{he} = t_h(1 + r_{he} r_{ee} r_{eh} r_{hh} + \ldots) r_{he} t_e = \frac{t_h r_{he} t_e}{1 - r_{he} r_{ee} r_{eh} r_{hh}}$$

Due to particle-hole symmetry, $r_{hh}(E) = r_{ee}^*(-E) \simeq r_{ee}^*(0) = r^*$, $\tilde{r}_{he} = \frac{t_h r_{he} t_e}{1 - R r_{he} r_{eh}} = \frac{t_h r_{he} t_e}{1 - R r_{he}^2(E)}$ *(* r_{eh}=r_{he}, $R = |r|^2$*).*

Resonance condition:

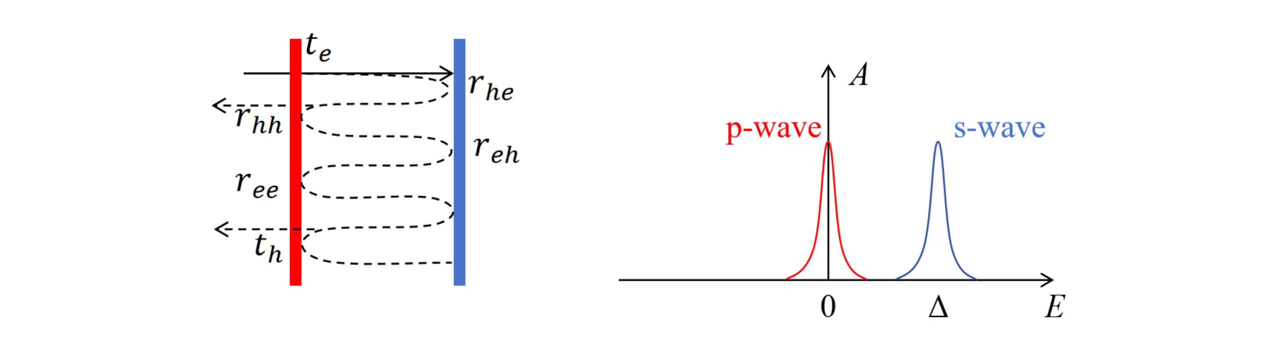
$$1 - R\, r_{he}^2(E) = 0$$

where $R \sim 1$ *(strong barrier). For s-wave superconductor,*

$$1 - e^{-2i\cos^{-1}(E/\Delta)} = 0, \Rightarrow 2\cos^{-1}(E/\Delta) = 0 \Rightarrow E = \Delta$$

For p-wave superconductor, $r_{eh} = -r_{he} = e^{i\pi} r_{he}$, *which leads to*

$$1 + e^{-2i\cos^{-1}(E/\Delta)} = 0 \Rightarrow 2\cos^{-1}(E/\Delta) = \pi \Rightarrow E = 0$$



3.3 Green's function

3.3.1 Introduction

S-matrix tells the response at one lead due to the excitation at another, e.g. t_{mn}. Green's function (GF): tells the response at at any point (inside or outside the conductor) due to an excitation at any other. For non-interaction transport, GF is a practical tool for computing S-matrix. More powerful dealing with interactions: $D_{op}E = S$, where D_{op} is a differential operator, R is the response, S is the excitation. Our problem: $[E-H_{op}]\psi = S$, where E is an energy parameter, not eigenenergy. H_{op} is the Hamiltonian. The Green operator: $G = [E - H_{op}]^{-1}$.

3.3.2 Retarded and Advanced GF

The inverse of a differential operator is not uniquely specified till we specify the boundary conditions. Start from the time-dependent Schrodinger equation,

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle, \quad |\psi(t)\rangle = \hat{U}(t,t')|\psi(t')\rangle \tag{3.200}$$

where U is the time-evolution operator. For time-independent $\hat{H}$, $\hat{U}(t,t') = e^{-i(t-t')\hat{H}/\hbar}$. For eigenstates $|\psi_n\rangle$,

$$\begin{aligned}\hat{U}(t,t') = e^{-i(t-t')\hat{H}/\hbar}\sum_n|\psi_n\rangle\langle\psi_n| = \sum_n e^{-iE_n(t-t')/\hbar}|\psi_n\rangle\langle\psi_n| \\ \Rightarrow |\psi(t)\rangle = \hat{U}(t,t')|\psi(t')\rangle = \sum_n e^{-iE_n(t-t')/\hbar}\langle\psi_n|\psi(t')|\psi_n\rangle\end{aligned} \tag{3.201}$$

Green operators: retarded:

$$\hat{G}^R(t,t') = -\frac{i}{\hbar}\theta(t-t')\hat{U}(t,t') = -\frac{i}{\hbar}\theta(t-t')e^{-i(t-t')\hat{H}/t} \tag{3.202}$$

advanced:

$$\hat{G}^A(t,t') = \frac{i}{\hbar}\theta(t'-t)\hat{U}(t,t') = \frac{i}{\hbar}\theta(t'-t)e^{-i(t-t')\hat{H}/t} \tag{3.203}$$

For $t > t'$,

$$|\psi(t)\rangle = i\hbar\hat{G}^R(t,t')|\psi(t')\rangle \tag{3.204}$$

For $t < t'$,

$$|\psi(t)\rangle = -i\hbar\hat{G}^A(t,t')|\psi(t')\rangle \tag{3.205}$$

For $t < t'$, $G^R(t,t') = 0$; for $t > t'$, $G^A(t,t') = 0$.

$$hatG^{R\dagger}(t,t') = \frac{i}{\hbar}\theta(t-t')e^{i(t-t')\hat{H}/\hbar} = \frac{i}{\hbar}\theta(t-t')e^{-i(t'-t)\hat{H}/\hbar} = \hat{G}^A(t',t) \tag{3.206}$$

$\hat{G}^R, \hat{G}^A$ satisfy the same equation:

$$(i\hbar\partial_t - \hat{H})\hat{G}^{R,A}(t,t') = \hat{I}\delta(t-t') \tag{3.207}$$

Remark $E(\omega) \to \hat{E} = i\hbar\partial_t$ as operator in the t representation.

$$\langle t|(E-\hat{H})\hat{G}|t'\rangle = \langle t|t'\rangle \Rightarrow (i\hbar\partial_t - \hat{H})\hat{G}(t,t') = \hat{I}\delta(t-t') \tag{3.208}$$

Check:

$$\begin{aligned}(i\hbar\partial_t - \hat{H})\hat{G}^R(t,t') &= \delta(t-t')e^{-i(t-t')\hat{H}/\hbar} - \frac{i}{\hbar}\hat{H}\theta(t-t')e^{-i(t-t')\hat{H}/\hbar} \\ &+\frac{i}{\hbar}\hat{H}\theta(t-t')e^{-i(t-t')\hat{H}/\hbar} = \delta(t-t')\hat{I}\end{aligned} \tag{3.209}$$

For $t > t'$, $|\psi(t)\rangle = i\hbar\hat{G}^R(t,t')|\psi(t')\rangle$,

$$i\hbar\partial_t|\psi(t)\rangle = (i\hbar)^2\frac{\partial}{\partial t}\hat{G}^R(t,t')|\psi(t')\rangle = i\hbar(\hat{H}\hat{G}^R + \delta(t-t')\hat{I})|\psi(t')\rangle = \hat{H}|\psi(t)\rangle \tag{3.210}$$

Time-independent Hamiltonian: $G(t,t') = G(t-t') = G(\tau)$, Fourier transform:

$$\hat{G}^{R(A)}(E) = \int_{-\infty}^{\infty}\hat{G}^{R(A)}(\tau)e^{iE\tau/\hbar}d\tau \tag{3.211}$$

To ensure convergence of the integral, we introduce $\eta = 0^+$,

$$\hat{G}^R(E) = \lim_{\eta\to 0}\int_{-\infty}^{\infty}\hat{G}^R(\tau)e^{i(E+i\eta)\tau/\hbar}d\tau \tag{3.212}$$

which converges at $\tau \to +\infty$,

$$\hat{G}^A(E) = \lim_{\eta\to 0}\int_{-\infty}^{\infty}\hat{G}^A(\tau)e^{i(E-i\eta)\tau/\hbar}d\tau \tag{3.213}$$

which converges at $\tau \to -\infty$. Otherwise, $\hat{G}$ diverges. e.g. free electron,

$$\begin{aligned}\hat{G}^R(E) &= \int_{-\infty}^{\infty} -\frac{i}{\hbar}\theta(\tau)e^{-i(E_i-E)\tau/\hbar}d\tau = \int_0^{\infty} -\frac{i}{\hbar}d\tau e^{-i(E_i-E)\tau/\hbar} \\ &= \frac{e^{-(E_i-E)\tau/\hbar}}{E_i-E}\Big|_0^{\infty} = \frac{1}{E-E_i} - \frac{e^{i(E-E_i)\infty/\hbar}}{E-E_i}\end{aligned} \tag{3.214}$$

By replacing $E \to E + i\eta$,

$$G^R(E) = \frac{1}{E-E_i+i\eta} - \frac{e^{i(E+i\eta-E_i)\infty/\hbar}}{E-E_i+i\eta} = \frac{1}{E-E_i+i\eta} \tag{3.215}$$

Remark η can be absorbed into the definition of $G^{R(A)}$, such that $G^R(\tau) = -\frac{i}{\hbar}\theta(\tau)e^{-i\tau(E_i-i\eta)/\hbar}$. At any finite τ, $\tau\cdot\eta = 0$, no effect; but for infinite τ, $\delta\tau = \infty, G^R(\tau\to\infty) = 0$. This modification of $G^{R/A}$ has no physical significance, since τ is always finite in the physically relevant regime. However, it is mathematically very convenient, because it allows us to work with well-define integrals. The divergence at $\tau = \infty$ has no physical effect.

Fourier transform:

$$\begin{aligned}(i\hbar\partial_t - \hat{H})\hat{G}^{R,A}(t,t') = \hat{I}\delta(t-t') &\Rightarrow \int_{\infty}^{\infty} d\tau e^{i(E+i\eta)\tau/\hbar}[i\hbar\frac{\partial}{\partial\tau}\hat{G}^R(\tau) - \hat{H}\hat{G}^R(\tau)] = \hat{I} \\ i\hbar[e^{i(E+i\eta)\tau/\hbar}\hat{G}^R(\tau)]|_{-\infty}^{\infty} - i\hbar\int d\tau[\frac{i(E+i\eta)}{\hbar}&e^{i(E+i\eta)\tau/\hbar}\hat{G}^R(\tau)] - \hat{H}\hat{G}^R(E)] = \hat{I}\end{aligned} \tag{3.216}$$

$$[E - i\eta - \hat{H}]\hat{G}^R(E) = \hat{I} \Rightarrow \hat{G}^R(E) = [(E+i\eta)\hat{I} - \hat{H}]^{-1} \tag{3.217}$$

Similarly,

$$\hat{G}^A(E) = [(E-i\eta)\hat{I} - \hat{H}]^{-1} \tag{3.218}$$

Eigen-basis:

$$\begin{aligned}\hat{G}^R(E) &= \frac{1}{(E+i\eta)\hat{I}-\hat{H}}\sum_n |\psi_n\rangle\langle\psi_n| = \sum_n \frac{|\psi_n\rangle\langle\psi_n|}{E-E_n+i\eta} \\ \hat{G}^R(\tau) &= \int_{-\infty}^{\infty}\hat{G}^R(E)e^{-iE\tau/\hbar}\frac{dE}{2\pi\hbar} = \sum_n\int_{-\infty}^{\infty}\frac{|\psi_n\rangle\langle\psi_n|}{E-E_n+i\eta}e^{-iE\tau/\hbar}\frac{dE}{2\pi\hbar}\end{aligned} \tag{3.219}$$

For $\tau > 0$,

$$\hat{G}^R(\tau) = \theta(\tau)\sum_n |\psi_n\rangle\langle\psi_n|e^{-i(E_n-i\eta)\tau/\hbar}(-2\pi i)\frac{dE}{2\pi\hbar} = -\frac{i}{\hbar}\theta(\tau)e^{-iE_n\tau/\hbar}|\psi_n\rangle\langle\psi_n| \tag{3.220}$$

3.3.3 GF in the coordinate representation

$$\begin{aligned}&\langle\vec{r}|\psi\rangle = \psi(\vec{r}),\ \langle\vec{r}|\hat{H}|\vec{r'}\rangle = \delta(\vec{r}-\vec{r'})\hat{H}(\vec{r'}),\ \langle\vec{r}|\hat{G}^R|\vec{r'}\rangle = G^R(\vec{r},\vec{r'}),\ |\psi(t)\rangle = i\hbar G^R(t-t')|\psi(t')\rangle \Rightarrow \\ &\psi(\vec{r},t) = \langle\vec{r}|\psi(t)\rangle = i\hbar\int d\vec{r'}\langle\vec{r}|\hat{G}^R|\vec{r'}\rangle\langle\vec{r'}|\psi(t')\rangle = i\hbar\int d\vec{r'}G^R(\vec{r}t,\vec{r'}t')\psi(\vec{r'},t')\end{aligned} \tag{3.221}$$

Time domain GF: $[i\hbar\partial_t - \hat{H}]\hat{G}^R(t,t') = \hat{I}\delta(t-t')$,

$$\langle\vec{r}|i\hbar\partial_t\hat{G}^R(t,t') - \hat{H}\hat{G}^R(t,t')|\vec{r'}\rangle = \delta(t-t')\delta(\vec{r}-\vec{r'}) \tag{3.222}$$

$$\begin{aligned}&i\hbar\partial_t\hat{G}^R(\vec{r}t,\vec{r'}t') - \hat{H}(\vec{r})\hat{G}^R(\vec{r}t,\vec{r'}t') = \delta(t-t')\delta(\vec{r}-\vec{r'}) \\ &\Rightarrow [i\hbar\partial_t - \hat{H}(\vec{r})]\hat{G}^R(\vec{r}t,\vec{r'}t') = \delta(t-t')\delta(\vec{r}-\vec{r'})\end{aligned} \tag{3.223}$$

where $\hat{H}(\vec{r}) = -\frac{\hbar^2\nabla^2}{2m} + V(\vec{r})$ is the single-particle Hamiltonian. Frequency domain GF:

$$[(E+i\eta)\hat{I}-\hat{H}]\hat{G}^R(E) = \hat{I} \Rightarrow [E+i\eta-\hat{H}(r)]G^R(\vec{r},\vec{r'},E) = \delta(\vec{r}-\vec{r'}) \tag{3.224}$$

(i) 1D free electron,

$$[E \pm i\eta + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}]G^{R,A}(x,x',E) = \delta(x-x') \tag{3.225}$$

Two exact solution:

$$G_1(x-x',E) = -\frac{im}{\hbar^2 k}e^{ik|x-x'|} = G^R \tag{3.226}$$

corresponding to "+",

$$G_2(x-x',E) = \frac{im}{\hbar^2 k}e^{-ik|x-x'|} = G^A \tag{3.227}$$

corresponding to "−", where

$$\hbar k = \sqrt{2m(E\pm i\eta)} = \sqrt{2mE}(1+\frac{i\eta}{E})^{1/2} \simeq \sqrt{2mE}(1\pm\frac{i\eta}{2E}) = \sqrt{2mE}(1\pm i\eta) \tag{3.228}$$

Apart from $x = x'$, trial function: $A^{\pm}e^{\pm ik(x-x')}$. At $x = x'$,

$$\begin{cases}\dfrac{\hbar^2}{2m}\displaystyle\int_{x'-0}^{x'+0}\frac{\partial^2}{\partial x^2}G(x,x',E)dx = 1 \\ \dfrac{\hbar^2}{2m}[G'(x'+0^+,x',E) - G'(x'-0^+,x',E)] = 1\end{cases}$$

gives boundary conditions (BC):

$$\begin{cases}G'(x'+0^+,x',E) - G'(x'-0^+,x',E) = \dfrac{2m}{\hbar^2} \\ G(x'+0^+,x',E) = G(x'-0^+,x',E)\end{cases}$$

Two possibility: $\pm k$ in different regions, otherwise no solution satisfies BC. G^R: for $x > x'$, $G(x,x') = A^+e^{ik(x-x')}$. For $x < x'$, $G(x,x') = A^-e^{-ik(x-x')}$.

$$ik(A^+ + A^-) = \frac{2m}{\hbar^2},\ A^+ = A^- \Rightarrow A^+ = A^- = \frac{m}{i\hbar^2 k} = -\frac{i}{\hbar v} \Rightarrow G(x,x',E) = \frac{i}{\hbar v}e^{ik|x-x'|} = G^R \tag{3.229}$$

Similarly, $G^A = \frac{i}{\hbar v} e^{-ik|x-x'|}$. Different BC: $G^R \to$ outgoing waves, $G^A \to$ incoming waves.

(ii) GF for a multi-moded wire G^R. Transverse mode $\chi_m(y)$ satisfy

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + U(y)]\chi_m(y) = \varepsilon_{m,0}\chi_m(y) \tag{3.230}$$

Orthogonality: $\int \chi_n(y)\chi_m(y)dy = \delta_{mn}$ (Assume χ_m real).

$$[E - U(y) + \frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2})]G_E(x, y, x', y') = \delta(x - x')\delta(y - y') \tag{3.231}$$

Eigenstate expansion: for $x > x'$,

$$G_E^R(x, y; x', y') = \sum_m A_m^+(y')\chi_m(y)e^{ik_m(x-x')} \tag{3.232}$$

For $x < x'$,

$$G_E^R(x, y; x', y') = \sum_m A_m^-(y')\chi_m(y)e^{-ik_m(x-x')} \tag{3.233}$$

where

$$G_E^{R'}(x' + 0^+, y, x', y') - G_E^{R'}(x' - 0^+, y, x', y') = \frac{2m}{\hbar^2}\delta(y - y') \tag{3.234}$$

$\frac{\hbar^2 k_m^2}{2m} = E - \varepsilon_{m,0}$. BC in x-direction:

$$G^R(x'+0^+, y, x', y') = G^R(x'-0^+, y, x', y') \Rightarrow \sum_m ik_m[A_m^+ + A_m^-]\chi_m(y) = \frac{2m}{\hbar^2}\delta(y-y')\int \chi_n dy \tag{3.235}$$

$$\sum_m A_m^+(y')\chi_m(y) = \sum_m A_m^-(y')\chi_m(y) \Rightarrow ik_m[A_m^+ + A_m^-] = \frac{2m}{\hbar^2}\chi_m(y') \tag{3.236}$$

$A_m^+(y') = A_m^-(y') \Rightarrow A_m^+ = A_m^- = -\frac{i}{\hbar v_m}\chi_m(y') \Rightarrow$

$$G_E^R(x, y; x', y') = \sum_m -\frac{i}{\hbar v_m}\chi_m(y)\chi_m(y')e^{ik_m|x-x'|} \tag{3.237}$$

Eigen-function expansion:

$$\begin{aligned} G^R(\vec{r}, \vec{r'}) = \langle \vec{r}|\hat{G}^R|\vec{r'}\rangle &= \sum_{m,\beta}\langle \vec{r}|m, \beta\rangle \frac{1}{E - \varepsilon_{m,0} - (\hbar^2\beta^2/2m) + i\eta}\langle m, \beta|\vec{r'}\rangle \\ &= \sum_{m,\beta}\frac{\psi_{m\beta}(r)\psi^*_{m\beta}(r')}{E - \varepsilon_{m,0} - (\hbar^2\beta^2/2m) + i\eta} \end{aligned} \tag{3.238}$$

where

$$\sum_\beta \to \frac{L}{2\pi}\int_{-\infty}^{\infty} d\beta, \psi_{m,\beta}(\vec{r}) = \frac{1}{\sqrt{L}}\chi_m(y)e^{i\beta x} \tag{3.239}$$

Thus

$$\begin{aligned} G^R(\vec{r}, \vec{r'}) &= \frac{1}{L}\sum_m \chi_m(y)\chi_m(y')\frac{L}{2\pi}\int d\beta \frac{e^{i\beta}(x - x')}{E - \varepsilon_{m,0} - (\hbar^2\beta^2/2m) + i\eta} \\ &= \frac{1}{L}\frac{2m}{\hbar^2}\sum_m \chi_m(y)\chi_m(y')\frac{L}{2\pi}\int d\beta \frac{e^{i\beta(x-x')}}{\frac{2m(E-\varepsilon_{m,0})}{\hbar^2} - \beta^2 + i\eta} \end{aligned} \tag{3.240}$$

Let $k_m^2 = \frac{2m(E-\varepsilon_{m,0})}{\hbar^2}$,

$$\begin{aligned} G^R(\vec{r}, \vec{r'}) &= -\frac{m}{\pi\hbar^2}\sum_m \chi_m(y)\chi_m(y')\int_{-\infty}^{\infty} d\beta \frac{e^{i\beta(x-x')}}{\beta^2 - k_m^2 - i\eta} \\ &= -\frac{m}{\pi\hbar^2}\sum_m \chi_m(y)\chi_m(y')\int_{-\infty}^{\infty} d\beta \frac{e^{i\beta(x-x')}}{(\beta - \beta_+)(\beta - \beta_-)} \end{aligned} \tag{3.241}$$

where $\beta_\pm = \pm\sqrt{k_m^2 + i\eta}$. For $x > x'$,

$$G^R(\vec{r};\vec{r'}) = -\frac{m}{\pi\hbar}\sum_m \chi_m(y)\chi_m(y')(2\pi i)\frac{e_+^\beta(x-x')}{\beta_+ - \beta_-} = \sum_m -\frac{im}{\hbar^2\beta_+}\chi_m(y)\chi_m(y')e^{i\beta_+(x-x')}$$
$$= \sum_m -\frac{i}{\hbar v_m}\chi_m(y)\chi_m(y')e^{ik_m(x-x')} \tag{3.242}$$

For $x < x'$,

$$G^R(\vec{r};\vec{r'}) = -\frac{m}{\pi\hbar}\sum_m \chi_m(y)\chi_m(y')(-2\pi i)\frac{e_-^\beta(x-x')}{\beta_- - \beta_+} = \sum_m -\frac{i}{\hbar v_m}\chi_m(y)\chi_m(y')e^{-ik_m(x-x')} \tag{3.243}$$

Thus

$$G^R(\vec{r};\vec{r'}) = \sum_m -\frac{i}{\hbar v_m}\chi_m(y)\chi_m(y')e^{ik_m|x-x'|} \tag{3.244}$$

Local density of states $\rho(\vec{r}, E)$:

$$\rho(\vec{r}, E) = \sum_n |\psi(\vec{r})|^2\delta(E-E_n), \quad G^R(\vec{r},\vec{r'},E) = \sum_n \frac{\langle\vec{r}|\psi_n\rangle\langle\psi_n|\vec{r'}\rangle}{E-E_n+i\eta} = \sum_n \frac{\psi_n(\vec{r})\psi_n^*(\vec{r'})}{E-E_n+i\eta} \tag{3.245}$$

Diagonal element:

$$G^R(\vec{r},\vec{r},E) = \sum_n \frac{|\psi_n(\vec{r})|^2}{E-E_n+i\eta} \tag{3.246}$$

$\frac{1}{x+i\eta} = P(\frac{1}{x}) - i\pi\delta(x) \Rightarrow$

$$\rho(\vec{r}, E) = \sum_n \delta(E-E_n)|\psi_n(\vec{r})|^2 = \frac{1}{\pi}\text{Im}[G^R(\vec{r},\vec{r},E)] \tag{3.247}$$

3.3.4 Lippmann-Schwinger equation: Relate GF and scattering theory

The advantage of GF is to interpret the theory using perturbation method. $\hat{H} = \hat{H}_0 + \hat{V}$, $\hat{H}_0$ is the kinetic energy of free particles in the leads. $\hat{V}$ is the scattering potential as perturbation that describe scattering.

$$\left[i\hbar\partial_t - \hat{H}_0 - \hat{V}_0\right]\hat{G}^R(t,t_0) = \hat{I}\delta(t-t_0)$$
$$[i\hbar\partial_t - \hat{H}_0]\hat{G}_0^R(t,t_1) = \hat{I}\delta(t-t_1) \tag{3.248}$$

$$i\hbar\partial_t - \hat{H}_0 = \hat{G}_0^{R^{-1}}(t,t_1)\delta(t-t_1) \Rightarrow \hat{G}_0^{R^{-1}}(t,t_1)\delta(t-t_1)\hat{G}^R(t,t_0) - \hat{V}\hat{G}^R(t,t_0) = \hat{I}\delta(t-t_0) \tag{3.249}$$

$$\hat{G}_0^{R^{-1}}(t_1,t)\delta(t-t_1)\hat{G}^R(t,t_0) - \hat{V}\hat{G}^R(t,t_0) = \hat{I}\delta(t-t_0)$$
$$\Rightarrow \delta(t-t_1)\hat{G}^R(t,t_0) - \hat{G}^R(t_1,t)\hat{V}\hat{G}^R(t,t_0) = \hat{G}_0^R(t_1,t)\delta(t-t_0)$$
$$\Rightarrow \hat{G}^R(t_1,t_0) - \int_{-\infty}^{\infty}\hat{G}_0^R(t_1,t)\hat{V}\hat{G}_0^R(t,t_0)dt = \hat{G}_0^R(t_1,t_0) \tag{3.250}$$

which leads to the Lippmann-Schwinger equation for GF:

$$G^R(t_1,t_0) = \hat{G}_0^R(t_1,t_0) + \int_{t_0}^{t_1}\hat{G}_0^R(t_1,t)\hat{V}\hat{G}^R(t,t_0)dt \tag{3.251}$$

change t:

$$G^R(t,t_0) = \hat{G}_0^R(t,t_0) + \int_{t_0}^{t}\hat{G}_0^R(t,t')\hat{V}\hat{G}^R(t',t_0)dt' \tag{3.252}$$

Formally

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{V}\hat{G} = \hat{G}_0 + \hat{G}_0\hat{V}(\hat{G}_0 + \hat{G}_0\hat{V}\hat{G}) = \hat{G}_0 + \hat{G}_0\hat{V}\hat{G} + \hat{G}_0\hat{V}\hat{G}_0\hat{V}\hat{G}_0 + \ldots$$
$$\hat{G} = \hat{G}_0 + (\hat{G}_0 + \hat{G}_0\hat{V}\hat{G}_0 + \ldots)\hat{V}\hat{G}_0 = \hat{G}_0 + \hat{G}\hat{V}\hat{G}_0 \tag{3.253}$$

which leads to

$$G^R(t,t_0) = \hat{G}_0^R(t,t_0) + \int_{t_0}^{t} \hat{G}^R(t,t')\hat{V}\hat{G}_0^R(t',t_0)dt' \tag{3.254}$$

Relate the GF to scattering states. Incoming state: time evolution of the initial state $\psi_0(t_0)$ from the past under the action of unperturbed Hamiltonian (G_0),

$$|\psi^{in}(t)\rangle = i\hbar \lim_{t_0\to-\infty} \hat{G}_0^R(t-t_0)|\psi_0(t_0)\rangle \tag{3.255}$$

Full scattering state: full Hamiltonian (G),

$$|\psi(t)\rangle = i\hbar \lim_{t_0\to-\infty} \hat{G}^R(t-t_0)|\psi_0(t_0)\rangle \tag{3.256}$$

Using Eq. (3.253) yields the Lippmann-Schwinger equation for the wave function:

$$\begin{aligned} |\psi(t)\rangle &= |\psi^{in}(t)\rangle + \int_{-\infty}^{\infty} dt' \hat{G}^R(t-t')\hat{V}|\psi^{in}(t')\rangle \\ \text{or} \quad |\psi(t)\rangle &= |\psi^{in}(t)\rangle + \int_{-\infty}^{\infty} dt' \hat{G}_0^R(t-t')\hat{V}|\psi(t')\rangle \end{aligned} \tag{3.257}$$

The corresponding Lippmann-Schwinger equation in the frequency-domain:

$$\begin{aligned} \hat{G}^R(E) &= \hat{G}_0^R(E) + \hat{G}^R(E)\hat{V}\hat{G}_0^R(E) \\ |\psi_E\rangle &= |\psi_E^{in}\rangle + \hat{G}^R(E)\hat{V}|\psi_E^{in}\rangle \\ \text{or} \quad \hat{G}^R(E) &= \hat{G}_0^R(E) + \hat{G}_0^R(E)\hat{V}\hat{G}^R(E) \\ |\psi_E\rangle &= |\psi_E^{in}\rangle + \hat{G}_0^R(E)\hat{V}|\psi_E\rangle \end{aligned} \tag{3.258}$$

in the coordinate representation:

$$\begin{aligned} \psi_E(\vec{r}) &= \psi_E^{in}(\vec{r}) + \int d\vec{r'} G^R(\vec{r},\vec{r'},E)V(\vec{r'})\psi_E^{in}(\vec{r'}) \\ \text{or} \quad \psi_E(\vec{r}) &= \psi_E^{in}(\vec{r}) + \int d\vec{r'} G_0^R(\vec{r},\vec{r'},E)V(\vec{r'})\psi_E(\vec{r'}) \end{aligned} \tag{3.259}$$

we express the wave function as a superposition of incoming + outgoing waves.

The Lippmann-Schwinger equation is useful in free space with localized scattering region or in rather simple geometries, when the unperturbed GF can be easily defined analytically. Consider the scattering at the δ-potential $V(x) = \alpha\delta(x)$ with incoming state specified as $\psi^{in}(x) = e^{ikx}$ (a given boundary condition), $G_0^R(x-x',E) = -\frac{im}{\hbar^2 k}e^{ik|x-x'|} \Rightarrow \psi(x) = e^{ikx} + \int dx'(\frac{-im}{\hbar^2 k})e^{ik|x-x'|}\alpha\delta(x')\psi(x') = e^{ikx} - \frac{im\alpha}{\hbar^2 k}e^{ik|x|}\psi(0)$. Inserting

$$\psi(x) = A\begin{cases} e^{ikx} + re^{-ikx} & x<0 \\ te^{ikx} & x>0 \end{cases}$$

for $x = 0^+, 0^-$,

$$\psi(x) = A\begin{cases} 1+r = 1 - \dfrac{im\alpha}{\hbar^2 k}(1+r) \\ t = 1 - \dfrac{im\alpha}{\hbar^2 k}t \end{cases}$$

This yields the right solution, meaning that the Lippmann-Schwinger equation provides the correct boundary condition.

Remark The Lippmann-Schwinger equation is generally useless in solving specific scattering problems. Its value is providing a general framework that relates the GF to the scattering states.

Exercise 3.6 (E.3.2, page 171) Derive Eq. 3.3.15 for the Green's function of an infinite wire using the eigenfunction expansion Eq. 3.3.17.

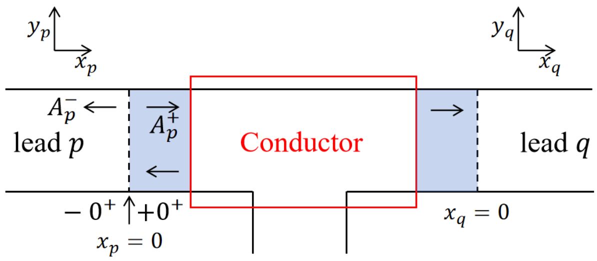
Eq. 3.3.15 in the book:

$$G_E^R(x,y;x',y') = \sum_m -\frac{i}{\hbar v_m}\chi_m(y)\chi_m(y')e^{ik_m|x-x'|}$$

where $k_m = \frac{\sqrt{2m(E-\varepsilon_{m,0})}}{\hbar}$ and $v_m = \frac{\hbar k_m}{m}$, Eq. 3.3.17 in the book:

$$G^R(\vec{r},\vec{r}') = \sum_\alpha \frac{\psi_\alpha(\vec{r})\psi_\alpha^*(\vec{r}')}{E-\varepsilon_\alpha+i\eta}$$

3.4 Fisher-Lee Relation: Express S-matrix by Green's function



$G_{pq}^R(y_q,y_p) = G_R(x_q=0,y_q;x_p=0^+,y_p)$, GF between points lying on $x_p=0$ and $x_q=0$. Formally, we have: $G_{pq}^R = \delta pq A_p^- + S'_{qp}A_p^+$, where S'_{qp} is the scattering amplitudes, net current amplitudes, and A_p^+ is the incoming amplitude.

Remark GF is related to the wave function, which does not involve the information of velocities. GF relates the planes $x_p=0$, $x_q=0$, including the places in the blue region. the S-matrix relates scattering waves incident from or outgoing to infinities, GF corresponds to excitation in the central region. Therefore, when we interpret scattering waves extending to infinities by GF, it must involve the A_p^- amplitude, and should be finally dropped.

For 1D case, $A_p^+ = A_p^- = -\frac{i}{\hbar v_p}$, $S'_{pq} = S_{pq}\sqrt{v_p/v_q}$ (S_{pq} is unitary)$\Rightarrow$

$$G_{pq}^R = -\frac{i}{\hbar v_p}\delta_{pq} - \frac{i}{\hbar v_p}\delta_{pq}S_{pq}\sqrt{v_p/v_q} \Rightarrow S_{qp} = -\delta_{qp}\sqrt{v_q/v_p} + i\hbar v_p\sqrt{v_q/v_p}G_{qp}^R \tag{3.260}$$

$$S_{qp} = -\delta_{pq} + i\hbar\sqrt{v_p v_q}G_{qp}^R \tag{3.261}$$

which is the 1D single mode Fisher-Lee relation.

Multi-moded leads:

$$G_{qp}^R(y_q,y_p) = \sum_{m\in p}\sum_{n\in q}[\delta_{nm}A_m^- + S'_{nm}A_m^+]\chi_n(y_q) \tag{3.262}$$

This extension is straightforward by noting that the propagation between two sites are achieved along versions eigen-channels (m,n); and the S-matrix relates these channels. $A_m^+ = A_m^- = -\frac{i}{\hbar v_m}\chi_m(y_p)$, $S'_{nm} = S_{nm}\sqrt{v_m/v_n} \Rightarrow$

$$\begin{aligned} G_{pq}^R(y_p,y_q) &= \sum_{m\in p}\sum_{n\in q}[\delta_{nm}(-\frac{i}{\hbar v_m})\chi_m(y_p) + S_{nm}\sqrt{\frac{v_m}{v_n}}(-\frac{i}{\hbar v_m})\chi_m(y_p)]\chi_n(y_p) \\ &= \sum_{nm} -\frac{i}{\sqrt{v_n v_m}}\chi_n(y_p)[\delta_{nm}+S_{nm}]\chi_m(y_p) \end{aligned} \tag{3.263}$$

Remark Again, at the scattering level, there is no mathematical difference between leads labels and channel labels.

Note that specifying m, n has specified the p and q lead. To interpret S-matrix by GF,

$$\begin{aligned}
&\iint \chi_n(y_q)[G^R_{pq}(y_q, y_p)]\chi_m(y_p)dy_p dy_q \\
&= -\frac{i}{\hbar}\sum_{m'n'}\iint \chi_n(y_q)\chi_m(y_p)\frac{1}{\sqrt{v_{n'}v_{m'}}}\chi_{n'}(y_p)[\delta_{n'm'} + S_{n'm'}]\chi_{m'}(y_p)dy_q dy_p \\
&= -\frac{i}{\hbar}\sum_{m'n'}\delta_{nn'}\delta_{mm'}\frac{1}{\sqrt{v_{n'}v_{m'}}}[\delta_{n'm'} + S_{n'm'}] = -\frac{i}{\hbar}\frac{1}{\sqrt{v_n v_m}}[\delta_{nm} + S_{nm}]
\end{aligned} \tag{3.264}$$

which leads to the general Fisher-Lee relation:

$$S_{nm} = -\delta_{mn} + i\hbar\sqrt{v_n v_m}\iint \chi_n(y_q)[G^R_{qp}(y_q, y_p)]\chi_m(y_p)dy_q dy_p \tag{3.265}$$

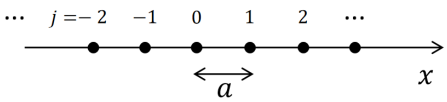
3.5 Tight-binding model (the method of finite differences)

Problems with arbitrarily shaped conductor, strategy: calculate GF (numerically), obtain S-matrix using Fisher-Lee relation, insert S-matrix to LB formula. Differential equation for GF:

$$[E - H_{op}(\vec{r}) + i\eta]G^R(\vec{r}, \vec{r'}) = \delta(\vec{r} - \vec{r'}), \quad H_{op}(\vec{r}) = \frac{(i\hbar\nabla + e\vec{A})^2}{2m} + U(\vec{r}) \tag{3.266}$$

Discretize the spatial coordinate: $G^R(\vec{r}, \vec{r'}) \to G^R(i, j)$ matrix $\Rightarrow [(E + i\eta)\hat{I} - \hat{H}]\hat{G}^R = \hat{I}$, where $[\hat{I}]$ is the identity matrix, $[\hat{H}]$ is the discretized Hamiltonian H_{op}. As long as we have the matrix $[(E + i\eta)\hat{I} - \hat{H}]$, then $\hat{G}^R$ can be obtained by inverting it.

Discretization



3.5.1 Matrix representation for H_{op} in 1D

$H_{op} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)$. Consider H_{op} acting on arbitrary function $F(x)$,

$$[H_{op}F(x)]_{x=ja} = \left[-\frac{\hbar^2}{2m}\frac{d^2F}{dx^2}\right]_{x=ja} + U_j F_j \tag{3.267}$$

where $F_j = F(x = ja), U_j = U(x = ja)$.

$$\begin{aligned}
&\left[\frac{d^2F}{dx^2}\right]_{x=ja} \to \frac{1}{a}\left\{\left[\frac{dF}{dx}\right]_{x=(j+\frac{1}{2})a} - \left[\frac{dF}{dx}\right]_{x=(j-\frac{1}{2})a}\right\} \to \frac{1}{a^2}(F_{i+1} - 2F_i + F_{i-1}) \\
&\Rightarrow [H_{op}F]_{x=ja} = (U_j + 2t)F_j - tF_{j-1} - tF_{j+1} = \sum_i H(j, i)F_i
\end{aligned} \tag{3.268}$$

where $t = \frac{\hbar^2}{2ma^2}$,

$$H = \begin{bmatrix}
\dots & -t & 0 & \dots & 0 \\
-t & U_{-1} + 2t & -t & \dots & 0 \\
0 & -t & U_0 + 2t & -t & \dots \\
\dots & \dots & \dots & \dots & \dots \\
0 & \dots & 0 & -t & \dots
\end{bmatrix} \tag{3.269}$$

Remark The continuous can be generally mapped to an artificial lattice (except for some Dirac models that breaking the no-go theorem). In this case, the lattice is not real, and only the long-wavelength limit has the physical meaning. In other cases, we start with the correct lattice model for the physical system, such as graphene. Then the lattice itself has physical meaning, including both the low and high energy parts.

1D Lattice model: $U(x) = U_0$, $E = U_0 + 2t(1 - \cos ka)$. For $ka \ll 1$, $E \simeq U_0 + 2t \times \frac{1}{2}k^2a^2 = U_0 + \frac{\hbar^2 k^2}{2m}$. Velocity: $v = \frac{\partial E}{\hbar \partial k} = 2a^2 tk/\hbar = \hbar k/m$.

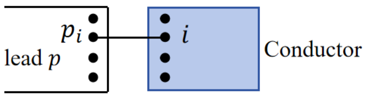
2D lattice: magnetic field $[H]_{ij} = U(\vec{r}_i) + \zeta t$ (ζ is the number of nearest neighbors)$= -\tilde{t}_{ij}$ (nearest-neighbor hopping).

Magnetic field: $\tilde{t}_{ij} = t\exp[ie\vec{A} \cdot (\vec{r}_i - \vec{r}_j)/\hbar]$, $\vec{A}$ is the magnetic vector potential (Peierls substitution).

Remark For artificial lattice to simulate the long-wavelength limit, the $\vec{B}$ is required to be smooth on the scale of the lattice constant.

3.5.2 Truncating the matrix

$\hat{G}^R = [(E + i\eta)\hat{I} - \hat{H}]^{-1}$, $\hat{H}$ is infinite dimensional. We are dealing with an open system connected to leads that extend to infinity. Trick: truncate the matrices properly by considering correct boundary condition.



The whole Hamiltonian $H = H_c + H_p + \tau_p$, where H_c is the conductor Hamiltonian, H_p is the Hamiltonian of lead p, τ_p is the coupling.

$$\hat{G} = \begin{bmatrix} G_p & G_{pc} \\ G_{cp} & G_c \end{bmatrix} = \begin{bmatrix} (E + i\eta)I - H_p & \tau_p \\ \tau_p^\dagger & EI - H_c \end{bmatrix}^{-1} \tag{3.270}$$

The discrete Hamiltonian H_c, H_p are determined by the physical system. Boundary term: $\tau_p(p_i, i) = t$. Derive the sub-matrix G_c, which corresponds to the effective theory for the conductor, taking into account the impact of the leads.

$$\begin{bmatrix} (E + i\eta)I - H_p & \tau_p \\ \tau_p^\dagger & EI - H_c \end{bmatrix} \begin{bmatrix} G_p & G_{pc} \\ G_{cp} & G_c \end{bmatrix} = I \tag{3.271}$$

which gives

$$\begin{cases} [(E + i\eta)I - H_p]G_p + \tau_p G_{cp} = I \\ [(E + i\eta)I - H_p]G_{pc} + \tau_p G_c = 0 \\ \tau_p^\dagger G_p + (EI - H_c)G_{cp} = 0 \\ \tau_p^\dagger G_{pc} + (EI - H_c)G_c = I \end{cases}$$

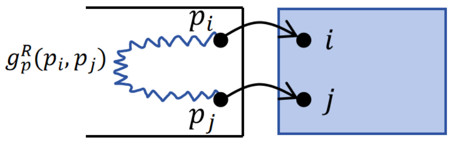
$\Rightarrow G_{pc} = -g_p^R \tau_p G_c$, where $g_p^R = [(E + i\eta)I - H_p]^{-1}$, bare GF of semi-infinite lead p.

$$[EI - H_c]G_c - \tau_p^\dagger g_p^R \tau_p G_c = I \Rightarrow G_c = [EI - H_c - \tau_p^\dagger g_p^R \tau_p]^{-1}, \quad H_c^{eff} = H_c + \tau_p^\dagger g_p^R \tau_p \tag{3.272}$$

Dimension of G_c: $C \times C$, C is the number of sites (taking into account other degrees of freedom such as spin, orbits, etc. in more complex cases). Infinite leads is taken into account exactly through the term $\Sigma_p^R = \tau_p^\dagger g_p^R \tau_p$, self-energy.

Problem: g_p^R still needs to invert an infinite matrix. Solution: g_p^R can be obtained in different ways, such as analytic calculation with proper boundary conditions. Matrix element of $\Sigma_p^R(i, j) = [\tau_p^\dagger g_p^R \tau_p]_{ij} = t^2 g_p^R(p_i, p_j)$.

Physical meaning of self-energy



Independent leads (otherwise combine them into a single one), $G_c = [EI - H_c - \Sigma^R]^{-1}$. Total self-energy $\Sigma^R = \sum_p \Sigma_p^R$, additive effect according to the physical pictures. Full GF $G_c = G_c^R$: propagation of electrons between two points inside the conductor, taking the effect of the leads into account through Σ^R.

Remark self-energy due to leads compared with self-energy due to e-e interaction, e-phonon interaction, etc.. Key difference: self-energy due to interaction is approximation, self-energy stemming from leads is exact. Another feature for self-energy is that generally, it is Non-Hermitian due to infinite leads. It indicates an mesoscopic platform for non-Hermitian physics.

Appendix: Proof of additivity of Σ_p^R:

$$\begin{bmatrix} g_{p_1}^{-1} & 0 & \dots & \dots & \tau_{p_1} \\ 0 & g_{p_2}^{-1} & 0 & \dots & \tau_{p_2} \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & g_{p_i}^{-1} & \tau_{p_i} \\ \tau_{p_1}^\dagger & \tau_{p_2}^\dagger & \dots & \tau_{p_i}^\dagger & EI - H_c \end{bmatrix} \begin{bmatrix} G_{p_1} & G_{p_1 P_2} & \dots & \dots & G_{p_1 c} \\ G_{p_2 P_1} & G_{p_2} & \dots & \dots & G_{p_2 c} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & G_{p_i} & G_{p_i c} \\ G_{cp_1} & G_{cp_2} & \dots & G_{cp_i} & G_c \end{bmatrix} = I \tag{3.273}$$

$$\begin{cases} g_{p_1}^{-1} G_{p_1 c} + \tau_{p_1} G_c = 0 \\ g_{p_2}^{-1} G_{p_2 c} + \tau_{p_2} G_c = 0 \\ \dots \\ g_{p_i}^{-1} G_{p_i c} + \tau_{p_i} G_c = 0 \end{cases}$$

which gives

$$G_{p_i c} = -g_{p_i} \tau_{p_i} G_c, \quad \tau_{p_1}^\dagger G_{p_1 c} + \tau_{p_2}^\dagger G_{p_2 c} + \dots + \tau_{p_i}^\dagger G_{p_i c} + (EI - H_c) G_c = I \tag{3.274}$$

$$(EI - H_c - \tau_{p_1}^\dagger g_{p_1} \tau_{p_1} - \tau_{p_2}^\dagger g_{p_2} \tau_{p_2} - \dots - \tau_{p_i}^\dagger g_{p_i} \tau_{p_i}) G_c = I \Rightarrow G_c = [EI - H_c - \sum_p \Sigma_p^R]^{-1} \tag{3.275}$$

What does the effective Hamiltonian mean? From the eigen-equation,

$$\begin{pmatrix} H_p & \tau_p \\ \tau_p^\dagger & H_c \end{pmatrix} \begin{pmatrix} \psi_p \\ \psi_c \end{pmatrix} = E \begin{pmatrix} \psi_p \\ \psi_c \end{pmatrix} \tag{3.276}$$

we derive the eigen-equation for ψ_c:

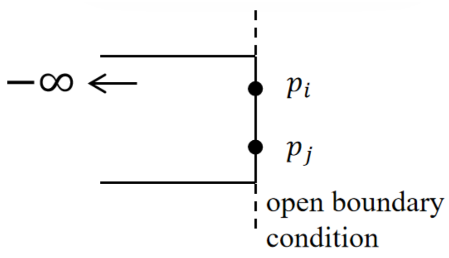
$$H_p \psi_p + \tau_p \psi_c = E \psi_p \Rightarrow (E - H_p) \psi_p = \tau_p \psi_c \Rightarrow \psi_p = g_p \tau_p \psi_c \tag{3.277}$$

$$\tau_p^\dagger \psi_p + H_c \psi_c = E \psi_c \Rightarrow (\tau_p^\dagger g_p \tau_p + H_c) \psi_c = H_{eff} \psi_c = E \psi_c \tag{3.278}$$

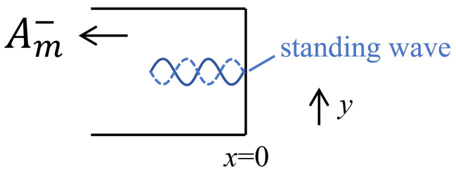
Note that H_{eff} is a function of E. If we solve the eigen-equation consistently, then we can obtain the eigen-energy of the whole system.

3.5.3 Solve the self-energy and transmission function

To obtain $\Sigma_p^R = \tau_p^\dagger g_p \tau_p + H_c$, we first solve g_p^R for an isolated lead. Goal: discrete



first solve a continuous semi-infinite wire



Appendix: Eigenfunction: $\psi_{m\beta} = \sqrt{\frac{2}{L}}\chi_m(y)\sin(\beta x)$, $\varepsilon_{m\beta} = \varepsilon_{m,0} + \frac{\hbar^2\beta^2}{2m}$. Expand GF using eigenfunction, $\hat{G}^R = \frac{1}{(E+i\eta)\hat{I}-\hat{H}}$:

$$\begin{aligned} G^R(\vec{r},\vec{r'}) &= \langle\vec{r}|\hat{G}^R|\vec{r'}\rangle = \langle\vec{r}|\frac{1}{(E+i\eta)\hat{I}-\hat{H}}|\vec{r'}\rangle = \sum_{m,\beta}\langle\vec{r}|m,\beta\rangle\frac{1}{E-\varepsilon_{m,\beta}+i\eta}\langle m,\beta|\vec{r'}\rangle \\ &= \sum_{m,\beta}\frac{\psi_{m\beta}(r)\psi^*_{m\beta}(r')}{E-\varepsilon_{m,0}-(\hbar^2\beta^2/2m)+i\eta} = \frac{2}{L}\sum_{m,\beta>0}\frac{\chi_m(y)\chi_m(y')\sin(\beta x)\sin(\beta x')}{E-\varepsilon_{m,0}-(\hbar^2\beta^2/2m)+i\eta} \end{aligned} \tag{3.279}$$

we focus on $x = x'$,

$$G^R(x,y,x',y') = \frac{2}{L}\sum_{m,\beta>0}\frac{\chi_m(y)\chi_m(y')\sin^2(\beta x)}{E-\varepsilon_{m,0}-(\hbar^2\beta^2/2m)+i\eta} \tag{3.280}$$

$\Delta\beta$(OBC)=$\frac{1}{2}\Delta k$(PBC), $\sum_\beta \to \frac{L}{\pi}\int d\beta \Rightarrow$

$$\begin{aligned}
G^R(x,y,x',y') &= \frac{2}{\pi}\sum_m \chi_m(y)\chi_m(y')\int_0^\infty \frac{\sin^2(\beta x)}{E-\varepsilon_{m,0}-(\hbar^2\beta^2/2m)+i\eta}d\beta \\
\sin^2(\beta x) &= (\frac{e^{i\beta x}-e^{-i\beta x}}{2i})^2 = \frac{2-e^{2i\beta x}-e^{-2i\beta x}}{4} \\
\Rightarrow G^R(\vec{r},\vec{r'}) &= \frac{1}{2\pi}\sum_m \chi_m(y)\chi_m(y')\int_0^\infty \frac{2-e^{2i\beta x}-e^{-2i\beta x}}{E-\varepsilon_{m,0}-(\hbar^2\beta^2/2m)+i\eta}d\beta \\
&= \frac{1}{2\pi}\sum_m \chi_m(y)\chi_m(y')\left[\int_{-\infty}^\infty \frac{1}{x}d\beta - \int_0^\infty \frac{e^{2i\beta x}}{x}d\beta - \int_0^\infty \frac{e^{-2i\beta x}}{x}d\beta\right] \\
&= \frac{1}{2\pi}\sum_m \chi_m(y)\chi_m(y')\left[\int_{-\infty}^\infty \frac{1}{x}d\beta - \int_{-\infty}^\infty \frac{e^{2i\beta x}}{x}d\beta\right] \\
&= \frac{1}{2\pi}\sum_m \chi_m(y)\chi_m(y')\left[\int_{-\infty}^\infty \frac{1-e^{2i\beta x}}{E-\varepsilon_{m,0}-(\hbar^2\beta^2/2m)+i\eta}d\beta\right] \\
&= -\frac{1}{2\pi}\sum_m \chi_m(y)\chi_m(y')\frac{2m}{\hbar^2}\left[\int_{-\infty}^\infty \frac{1}{\beta^2-k_m^2-i\eta}d\beta - \int_{-\infty}^\infty \frac{e^{2i\beta x}}{\beta^2-k_m^2-i\eta}d\beta\right] \\
&= -\frac{m}{\pi\hbar^2}\sum_m \chi_m(y)\chi_m(y')\left[\int_{-\infty}^\infty \frac{1}{(\beta-\beta_+)(\beta-\beta_-)}d\beta - \int_{-\infty}^\infty \frac{e^{2i\beta x}}{(\beta-\beta_+)(\beta-\beta_-)}d\beta\right] \\
&= -\frac{m}{\pi\hbar^2}\sum_m \chi_m(y)\chi_m(y')\left[\int_{-\infty}^\infty (\frac{1}{\beta-\beta_+}-\frac{1}{\beta-\beta_-})(\frac{1}{\beta_+-\beta_-})d\beta - \frac{(2\pi i)}{\beta_+-\beta_-}e^{2i\beta_+ x} + \frac{(2\pi i)}{\beta_--\beta_+}e^{2i\beta_- x}\right] \\
&= -\frac{m}{\pi\hbar^2}\sum_m \chi_m(y)\chi_m(y')\left[\int_{-\infty}^\infty (\frac{1}{\beta-k_m-i\eta}-\frac{1}{\beta+k_m+i\eta})\frac{1}{2k_m}d\beta - (2\pi i)\frac{1}{2k_m}e^{2ik_m x}\right] \\
&= -\frac{m}{\pi\hbar^2}\sum_m \chi_m(y)\chi_m(y')[2\pi i - 2\pi i e^{2ik_m x}]\frac{1}{2k_m} = -\sum_m \frac{i}{\hbar v_m}\chi_m(y)\chi_m(y')[1-e^{2ik_m x}] \\
&= \sum_m \frac{2\sin(k_m x)}{\hbar v_m}\chi_m(y)e^{ik_m x}\chi_m(y')
\end{aligned} \tag{3.281}$$

where $\beta_\pm = \pm(k_m+i\eta)$. $G^R(x,y,x',y') = \sum_m \frac{2\sin(k_m x)}{\hbar v_m}\chi_m(y)e^{ik_m x}\chi_m(y')$. Discrete version: $y=p_i$, $y'=p_j$, $x=a$, otherwise, $G^R=0$. Long-wavelength limit: $\sin k_m a \sim k_m a = v_m\frac{m}{\hbar}a = v_m\frac{\hbar}{2ta}$,

$$\tilde{g}^R(p_i,p_j) = -\sum_m \frac{1}{ta}\chi_m(p_i)e^{ik_m a}\chi_m(p_j) \tag{3.282}$$

Note that the above expression is not the final result. Special cares should be taken to the correspondence between the continuous and discrete quantities.

δ-function: $\delta(x)\to\frac{1}{a}\delta_{i,0}$. δ-function is defined by the integral $\int f(x)\delta(x)dx = f(0)$

$$\Rightarrow \sum_i \Delta x_i\delta(x_i)f(x_i) = \sum_i \delta_{i,0}f(x_i) = f(0) \Rightarrow \Delta x_i\delta(x_i) = \delta_{i,0} \tag{3.283}$$

or $\delta(x) = \frac{1}{a}\delta_{i,0}$ (Note $a=\Delta x_i$). For wave function $\psi(x)$, normalization requires

$$\int \psi^*(x)\psi(x)dx = 1 = \sum_i \psi^*(ia)\psi(ia)\Delta x_i = \sum_i \psi^*(ia)\psi(ia)a \tag{3.284}$$

Discrete:

$$\sum_i \widetilde{\psi}^*(i)\widetilde{\psi}(i) = 1 \Rightarrow \widetilde{\psi}(i) = \sqrt{a}\psi(ia) \tag{3.285}$$

Note that $G(x,x') = \sum_n \frac{\psi_n(x)\psi_n^*(x')}{E-E_n}$, so that the discrete 1D GF differs from the continuous GF by a, so

$$g^R(p_i,p_j) = a\tilde{g}^R = -\sum_m \frac{1}{t}\chi_m(p_i)e^{ik_m a}\chi_m(p_j) \tag{3.286}$$

which is the desired result, with the unit of E^{-1}. $g^R(p_i,p_j)$ is called surface GF, which is the GF elements at the surface sites, with the semi-infinity of the leads taken into account already by the boundary condition.

Remark In most cases, the surface GF cannot be solved in an analytic way. The iterative method is usually adopted for the discrete leads, see Ryndyk.

After we obtain the surface GF, we have the self-energy

$$\Sigma_p^R(i,j) = t^2 g^R(p_i,p_j) = -t\sum_{m\in p}\chi_m(p_i)e^{ik_m a}\chi_m(p_j) \tag{3.287}$$

3.5.4 Transmission function

Use the result of GF and the Fisher-Lee relation, we can calculate the S-matrix and so the transmission function. $S_{nm} = -\delta_{mn} + i\hbar\sqrt{v_n v_m}\iint \chi_n(y_q)[G_{qp}^R(y_q,y_p)]\chi_m(y_p)dy_q dy_p$. Discrete version: $\chi_n(y_q\to q_i)$, $\chi_n(y_p\to p_i)$, $G_{qp}^R(y_q\to j, y_p\to i)$. Specifically, $\sqrt{a}\chi_n(y_q=q_j a) = \chi_n(q_j)$, $\sqrt{a}\chi_m(y_p=p_i a) = \chi_m(p_i)$, $aG_{qp}^R(y_q=ja,y_p=ia,x,x') = G_{qp}^R(j,i,x,x')$, $a^2 G_{qp}^R(y_q,y_p,x,x') = G_{qp}^R(j,i,j_x,j_{x'})$.

$$\begin{aligned} S_{nm} &= -\delta_{mn} + i\hbar\sqrt{v_n v_m}\sum_{i,j}\Delta y_i\Delta y_j\chi_n(y_q=q_j a)[G^R(y_q=ja,y_p=ia)]\chi_m(y_p=p_i a) \\ &= -\delta_{mn} + i\hbar\sqrt{v_n v_m}\sum_{i,j}a^2\chi_n(y_q=q_j a)[G^R(y_q=ja,y_p=ia)]\chi_m(y_p=p_i a) \\ &= -\delta_{mn} + i\hbar\sqrt{v_n v_m}\sum_{i,j}\chi_n(q_j)\frac{G^R(j,i)}{a}\chi_m(p_i) \end{aligned} \tag{3.288}$$

The factor a comes from the discretization in the x-direction. The "a" factor does not matter for the y-direction. The integral and sum is equivalent as long as the correspondence of the wave functions are properly related.

For $n\neq m$, $\delta_{nm}=0$:

$$|S_{nm}|^2 = \frac{\hbar^2 v_n v_m}{a^2}\sum_{ijj'i'}\chi_n(q_j)G^R(j;i)\chi_m(p_i)\chi_m(p_{i'})G^R(j';i')\chi_n(q_{j'}) \tag{3.289}$$

$$= \sum_{ijj'i'}\chi_n(q_{j'})\frac{\hbar v_n}{a}\chi_n(q_j)G^R(j,i)\chi_m(p_i)\frac{\hbar v_m}{a}\chi_m(p_{i'})G^A(i',j') \tag{3.290}$$

$$\begin{aligned} \bar{T}_{qp} = \sum_{n\in q}\sum_{m\in p}|S_{nm}|^2 = \sum_{ijj'i'}\Bigg\{&\left[\sum_{n\in q}\chi_n(q_{j'})\frac{\hbar v_n}{a}\chi_n(q_j)\right]G^R(j,i) \\ &\times\left[\sum_{m\in p}\chi_m(p_i)\frac{\hbar v_m}{a}\chi_m(p_{i'})\right]G^A(i',j')\Bigg\} \end{aligned} \tag{3.291}$$

where $\left[\sum_{n\in q}\chi_n(q_{j'})\frac{\hbar v_n}{a}\chi_n(q_j)\right]$ is $\Gamma_q(j',j)$, and $\left[\sum_{m\in p}\chi_m(p_i)\frac{\hbar v_m}{a}\chi_m(p_{i'})\right]$ is $\Gamma_p(i,i')$.

so

$$\bar{T}_{qp} = \sum_{ijj'i'}\Gamma_q(j',j)G^R(j,i)\Gamma_p(i,i')G^A(i',j') = \mathrm{Tr}\left[\Gamma_q G^R\Gamma_p G^A\right] \tag{3.292}$$

This compact form is widely used, which generally holds in a broader context.

$\Gamma_p(i,j)$ is called line-width function, it is related to the self-energy as

$$\Gamma_p = i[\Sigma_p^R - \Sigma_{\bar{p}}^A] \tag{3.293}$$

$$\Sigma_p^R(i,j) = -t\sum_{m\in p}\chi_m(p_i)e^{ik_m a}\chi_m(p_j) \tag{3.294}$$

$$\Rightarrow i(\Sigma_p^R - \Sigma_p^A) = it\sum_{m\in p}\chi_m(p_i)(e^{-ik_m a} - e^{ik_m a})\chi_m(p_j) \tag{3.295}$$

$$= it\sum_{m\in p}\chi_m(p_i)(-2i)\sin k_m a\chi_m(p_j) \tag{3.296}$$

$$\simeq \sum_{m\in p}\chi_m(p_i)(2tv_m\frac{\hbar}{2ta})\chi_m(p_j) \tag{3.297}$$

$$= \sum_{m\in p}\chi_m(p_i)\frac{\hbar v_m}{a}\chi_m(p_j) = \Gamma_p(i,j) \tag{3.298}$$

Remark Although these relations are derived using the normal electron. the formula and physical results are more general, which can be derived in a rather general way, using NEGF.

Interpretation of $\bar{T}_{pq} = \mathrm{Tr}\left[\Gamma_q G^R \Gamma_p G^A\right]$:

- $G^{R,A}$: describes the dynamics of electrons inside the conductor, taking the effect of the leads into account through the self-energy $\Sigma^{R,A}$.
- Γ: describes the coupling of the conductor to the leads.

To understand it more clearly, lets focus on S_{nm} $(n \neq m)$:

$$S_{nm} = i\hbar\sqrt{v_n v_m}\sum_{ij}\chi_n(q_j)\frac{G^R(j;i)}{a}\chi_m(p_i) \tag{3.299}$$

Appendix for LDOS:

$$\psi_{m\beta}(x=0^+) = \sqrt{\frac{2}{L}}\chi_m(y)\sin(\beta x) \simeq \sqrt{\frac{2}{L}}\chi_m(y)\sin(\beta a) \simeq \sqrt{\frac{2}{L}}\chi_m(y)\beta x \tag{3.300}$$

LDOS for the m-mode:

$$\rho_m(x=0^+,y;E) = \sum_\beta \delta(E-E_{m\beta})\psi^*_{m\beta}(0^+)\psi_{m\beta}(0^+) \tag{3.301}$$

$$= \frac{L}{\pi}\int d\beta\,\delta(E-E_{m\beta})\frac{2}{L}\chi_m^2(y)\beta^2 a^2 = \frac{2}{\pi}\int d\beta\,\delta(E-E_{m\beta})\chi_m^2(y)\left(\frac{\hbar v_\beta}{2at}\right)^2 \tag{3.302}$$

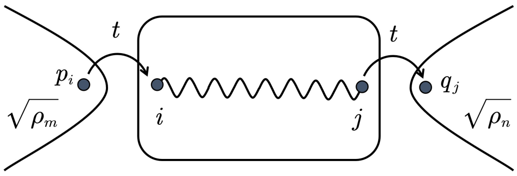
$$= \frac{2}{\pi}\int dE_{m\beta}\delta(E-E_{m\beta})\chi_m^2(y)\frac{\hbar v_\beta}{(2at)^2} \tag{3.303}$$

$$= \frac{2}{\pi}\chi_m^2(y)\frac{\hbar v_m(E)}{(2at)^2} \tag{3.304}$$

$$\Rightarrow \hbar v_m\chi_m^2 = \rho_m(0^+,y;E)\frac{\pi}{2}(2at)^2 \tag{3.305}$$

$$\Rightarrow \sqrt{\hbar v_m}\chi_m = \sqrt{\rho_m(0^+,y;E)}\sqrt{\frac{\pi}{2}}(2at) \propto \sqrt{\rho_m(p_i)}t \tag{3.306}$$

$$S_{nm} \propto \sum_{ij}\sqrt{\rho_n(q_j)}tG^R(j;i)t\sqrt{\rho_m(p_i)} \tag{3.307}$$



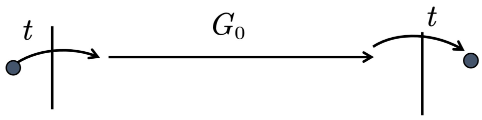
Dyson equation and Feynman paths:

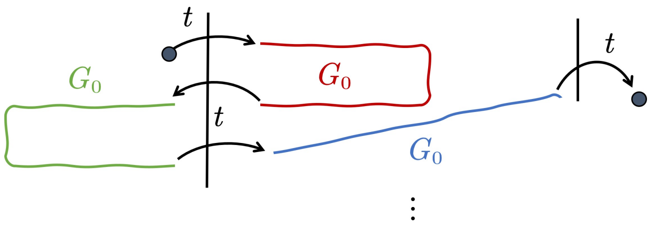
$$G^{R^{-1}} = E - H_c - \Sigma = G_0^{R^{-1}} - \Sigma \tag{3.308}$$

$$G^R = G_0^R + G_0^R \Sigma^R G^R = G_0^R + G_0^R \Sigma G_0^R + ... \tag{3.309}$$

$$\Rightarrow G^R(j;i) = G_0^R(j,i) + G_0^R(j,i')\Sigma(i',j')G_0^R(j',i) + ... \tag{3.310}$$

$$\Sigma(i,j) = \sum_p \Sigma_p \sum_p t g_p^R(p_i,p_j) t \tag{3.311}$$





3.5.5 An effective Non-Hermitian problem

$$G_c^{R^{-1}} = E - H_c - \Sigma^R = E - H_{eff}, \qquad H_{eff} = H_c + \Sigma^R \tag{3.312}$$

where $H_{eff}^\dagger \neq H_{eff}$ due to $\Sigma^{R\dagger} \neq \Sigma^R$ in general.

Eigen-equation for the effective Non-Hermitian:

$$H_{eff}\psi_\alpha = \varepsilon_\alpha \psi_\alpha \tag{3.313}$$

where $\{\varepsilon_\alpha\}$ are general complex, except for some PT mechanism.

$$\varepsilon_\alpha = \varepsilon_{\alpha 0} - \Delta_\alpha - i(\gamma_\alpha/2) \tag{3.314}$$

where $\varepsilon_{\alpha 0}$ is the eigen-energy of H_c, is real, and $-\Delta_\alpha - i(\gamma_\alpha/2)$ is correction due to leads.

$$\psi_\alpha(t) = e^{-i\varepsilon_\alpha at/\hbar}\psi_\alpha)(0) = e^{-i(\varepsilon_{\alpha 0}-\Delta_\alpha)t/\hbar} e^{-\frac{\gamma_\alpha}{2}t/\hbar}\psi_\alpha(0) \tag{3.315}$$

Δ_α is the renormalization of energy, γ_α captures the escape of electrons from the conductor to the leads.

Probability: $|\psi_\alpha|^2 e^{-\gamma_\alpha t\hbar}$, $\hbar/\gamma_\alpha$ is the lifetime inside the conductor. For isolated conductor, it's Hermitian, $\gamma_\alpha = 0$, with infinite lifetime.

3.5.6 Eigenfunction expansion: bi-orthonormal set

$$H_{eff}\psi_\alpha = \varepsilon_\alpha \psi_\alpha \tag{3.316}$$

where $\{\psi_\alpha\}$ do not form an orthogonal set. Consider the eigenstates Φ_α of the adjoint operator:

$$H^\dagger_{eff}\Phi_\alpha = \varepsilon^*_\alpha \Phi_\alpha \tag{3.317}$$

$\{\psi_\alpha\}$, $\{\Phi_\alpha\}$ form a bi-orthonormal set, $\{\psi_\alpha\}$ is called right basis, $\{\Phi_\alpha\}$ is the left one.

$$\int \Phi^*_\alpha(\vec{r})\psi_\beta(\vec{r})d\vec{r} = \delta_{\alpha\beta} \tag{3.318}$$

The Green's function naturally be expanded by the left-right basis as

$$\hat{G}^R = \frac{1}{E - H_{eff}} \sum_\alpha |\psi_\alpha\rangle \langle\Phi_\alpha| \tag{3.319}$$

$$= \sum_\alpha \frac{|\psi_\alpha\rangle \langle\Phi_\alpha|}{E - E_\alpha} \tag{3.320}$$

$$\Rightarrow G^R(\vec{r},\vec{r}') = \langle\vec{r}|\, \hat{G}^R \,|\vec{r}'\rangle = \sum_\alpha \frac{\psi_\alpha(\vec{r})\Psi^*_\alpha(\vec{r}')}{E - E_\alpha}, \qquad \gamma_\alpha > 0, \text{ no need of } \eta. \tag{3.321}$$

Remark The Green's function language can naturally deal with effective Non-Hermitian problem. Within this framework, the bi-orthonormal basis is adopted. Recent progress in Non-Hermitian physics inspires us to "engineer" the effective Non-Hermitian problem via proper leads[12] .

[12] See Shao PRL 2024, Geng PRB 2023.