Generalization of scattering problem in a quasi 1D

We consider a device connected to the left (Lead 1) and right (Lead 2) leads as depicted below.

It is assumed that electrons flow steadily from the left to right. Then, the time-dependent Schrödinger equation can be reduced to the following form.

$$\begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^{+} & H_D & \tau_2^{+} \\ 0 & \tau_2 & H_2 \end{pmatrix} \begin{pmatrix} |\psi_1\rangle \\ |\psi_d\rangle \\ |\psi_2\rangle \end{pmatrix} = E \begin{pmatrix} |\psi_1\rangle \\ |\psi_d\rangle \\ |\psi_2\rangle \end{pmatrix} \quad \cdots\cdots (1)$$

$H_1, H_d, H_2, \tau_1, \tau_2$ are all matrices

At the beginning, we assume that the Schrödinger eq. of the isolated lead 1 is solved as

$$H_1 |\phi_{in}\rangle = E |\phi_{in}\rangle \quad \cdots\cdots (2)$$

Then, we consider ϕ_{in} as incident wave to the device region. In the steady state, ψ can be expressed by the sum of incident and reflected waves as

$$|\psi\rangle = \begin{pmatrix} |\psi_1\rangle \\ |\psi_d\rangle \\ |\psi_2\rangle \end{pmatrix} = |\phi_{in}\rangle + |\chi\rangle = \begin{pmatrix} |\phi_{in}\rangle + |\chi_1\rangle \\ |\chi_d\rangle \\ |\chi_2\rangle \end{pmatrix} \quad \cdots\cdots (3)$$

By inserting Eq. (3) into Eq. (1), we have

$$\begin{pmatrix} E-H_1 & -\tau_1 & 0 \\ -\tau_1^\dagger & E-H_d & -\tau_2^\dagger \\ 0 & -\tau_2 & E-H_2 \end{pmatrix} \begin{pmatrix} |\phi_{in}\rangle + |\chi_1\rangle \\ |\chi_d\rangle \\ |\chi_2\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad \cdots (4)$$

$$\rightarrow \begin{pmatrix} E-H_1 & -\tau_1 & 0 \\ -\tau_1^\dagger & E-H_d & -\tau_2^\dagger \\ 0 & -\tau_2 & E-H_2 \end{pmatrix} \begin{pmatrix} |\chi_1\rangle \\ |\chi_d\rangle \\ |\chi_2\rangle \end{pmatrix} = \begin{pmatrix} -(E-H_1)|\phi_{in}\rangle \\ \tau_1^\dagger |\phi_{in}\rangle \\ 0 \end{pmatrix} \quad \cdots (5)$$

From Eq. (2), we see $-(E-H_1)|\phi_{in}\rangle = -(E-E)|\phi_{in}\rangle = 0$.

So, we have

$$\begin{pmatrix} |\chi_1\rangle \\ |\chi_d\rangle \\ |\chi_2\rangle \end{pmatrix} = G \begin{pmatrix} 0 \\ \tau_1^\dagger |\phi_{in}\rangle \\ 0 \end{pmatrix} \quad \cdots (6)$$

$$G = \begin{pmatrix} E-H_1 & -\tau_1 & 0 \\ -\tau_1^\dagger & E-H_d & -\tau_2^\dagger \\ 0 & -\tau_2 & E-H_2 \end{pmatrix}^{-1} = \begin{pmatrix} G_1 & G_{1d} & G_{12} \\ G_{d1} & G_d & G_{d2} \\ G_{21} & G_{2d} & G_2 \end{pmatrix} \quad \cdots (7)$$

From the second row in Eq. (6), we obtain

$$|\chi_d\rangle = G_d \tau_1^\dagger |\phi_{in}\rangle = |\psi_d\rangle \quad \cdots (8)$$

From the third row of Eq. (4), we have

$$(E - H_2)|\chi_2\rangle = \tau_2 |\chi_d\rangle$$

$g_2 = (E - H_2)^{-1}$

Note $g_2 \neq G_2$.

$$|\chi_2\rangle = (E - H_2)^{-1} \tau_2 |\chi_d\rangle = g_2 \tau_2 |\chi_d\rangle \quad \cdots\cdots (9)$$

Inserting Eq. (8) into Eq. (9), we obtain

$$|\chi_2\rangle = g_2 \tau_2 G_d \tau_1^{\dagger} |\phi_{in}\rangle = |\psi_2\rangle \quad \cdots\cdots (10)$$

From the first row of Eq. (5), we have

$$(E - H_1)|\chi_1\rangle = \tau_1 |\chi_d\rangle$$

$g_1 = (E - H_2)^{-1}$

$$|\chi_1\rangle = (E - H_1)^{-1} \tau_1 |\chi_d\rangle = g_1 \tau_1 |\chi_d\rangle \quad \cdots (11)$$

Inserting Eq (8) into Eq. (11) yields the following relation.

$$|\chi_1\rangle = g_1 \tau_1 G_d \tau_1^{\dagger} |\phi_{in}\rangle \quad \cdots\cdots (12)$$

From Eqs. (8), (10), and (12), we obtain

$$\boxed{\begin{aligned} |\psi_1\rangle &= (1 + g_1 \tau_1 G_d \tau_1^{\dagger}) |\phi_{in}\rangle \\ |\psi_d\rangle &= G_d \tau_1^{\dagger} |\phi_{in}\rangle \quad \cdots\cdots (13) \\ |\psi_2\rangle &= g_2 \tau_2 G_d \tau_1^{\dagger} |\phi_{in}\rangle \end{aligned}}$$

We see that ψ can be expressed by the incident wave ϕ_{in}.

If the scattering process occurs independly, we should consider the scattering process from the lead 2 to lead 1 equally.

Charge density in the device

From Eq. (13), we see that the wave function $\Psi_{d,n}^{(1)}$ $(= \Psi_d)$ is contributed by the incident wave ϕ_{1n} from the lead 1. So, the density operator of the device region can be defined by

$$\hat{\rho}_d^{(1)} = \int_{-\infty}^{\infty} dE \sum_n f(E,\mu_1)\, \delta(E-E_n)\, |\Psi_{d,n}^{(1)}\rangle\langle\Psi_{d,n}^{(1)}|$$

$$\overset{\text{Eq. (13)}}{=} \int_{-\infty}^{\infty} dE\, f(E,\mu_1) \sum_n \delta(E-E_n)\, G_d \tau_1^{+} |\phi_{1n}\rangle\langle\phi_{1n}| \tau_1 G_d^{+}$$

$$= \int_{-\infty}^{\infty} dE\, f(E,\mu_1)\, G_d \tau_1^{+} \underbrace{\left[\sum_n \delta(E-E_n)\, |\phi_{1n}\rangle\langle\phi_{1n}|\right]}_{\frac{a_1}{2\pi}} \tau_1 G_d^{+}$$

$$= \int_{-\infty}^{\infty} dE\, f(E,\mu_1)\, G_d \tau_1^{+} \frac{a_1}{2\pi} \tau_1 G_d^{+} \qquad \text{----- (14)}$$

By defining

$$\Gamma_1 = \tau_1^{+} a_1 \tau_1 \qquad \text{----- (15)}$$

we rewrite Eq. (14) as

This is called Non-Equilibrium Green's Function (NEGF).

$$\hat{\rho}_d^{(1)} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dE\, f(E,\mu_1)\, \underbrace{G_d \Gamma_1 G_d^{+}}_{\text{NEGF}} \qquad \text{----- (16)}$$

The matrix elements of $\hat{\rho}_d^{(1)}$ are evaluated by $\langle l | \hat{\rho}_d^{(1)} | m \rangle$ where $|l\rangle$ and $|m\rangle$ are basis functions in the device region. By considering all the contributions from all the leads connected to the device, we obtain

spin degeneracy

$$\boxed{\hat{\rho} = \frac{2}{2\pi} \int_{-\infty}^{\infty} dE \left[\sum_i f(E,\mu_i)\, G_d \Gamma_i G_d^{+}\right]} \qquad \text{----- (17)}$$

Current through the device

In the non-equilibrium steady state the probability density of the device region is conserved. We evaluate the flux of the probability density using the time-dependent Schrödinger equation as

$$i\hbar \frac{\partial}{\partial t}\begin{pmatrix} |\psi_1\rangle \\ |\psi_d\rangle \\ |\psi_2\rangle \end{pmatrix} = \begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^+ & H_d & \tau_2^+ \\ 0 & \tau_2 & H_2 \end{pmatrix}\begin{pmatrix} |\psi_1\rangle \\ |\psi_d\rangle \\ |\psi_2\rangle \end{pmatrix} \quad \cdots\cdots (18)$$

The time evolution of the integrated probability density is given by

$$\frac{\partial}{\partial t}\langle\psi_d|\psi_d\rangle = \frac{\partial\langle\psi_d|}{\partial t}|\psi_d\rangle + \langle\psi_d|\frac{\partial|\psi_d\rangle}{\partial t}$$

← From Eq. (18)

$$= \frac{i}{\hbar}\left[\langle\psi_2|\tau_2 + \langle\psi_d|H_d + \langle\psi_1|\tau_1\right]|\psi_d\rangle$$

$$- \frac{i}{\hbar}\langle\psi_d|\left[\tau_1^+|\psi_1\rangle + H_d|\psi_d\rangle + \tau_2^+|\psi_2\rangle\right]$$

$$= \frac{i}{\hbar}\left[\left(\langle\psi_1|\tau_1|\psi_d\rangle - \langle\psi_d|\tau_1^+|\psi_1\rangle\right) + \left(\langle\psi_2|\tau_2|\psi_d\rangle - \langle\psi_d|\tau_2^+|\psi_2\rangle\right)\right] \quad \cdots\cdots (19)$$

Each term in Eq. (19) can be regarded as the contribution from each lead k.

The flow of current is opposite to that of electron

This is purely imaginary.

$$i_k = -\frac{ie}{\hbar}\left(\underbrace{\langle\psi_k|\tau_k|\psi_d\rangle - \langle\psi_d|\tau_k^+|\psi_k\rangle}\right) \quad \cdots\cdots (20)$$

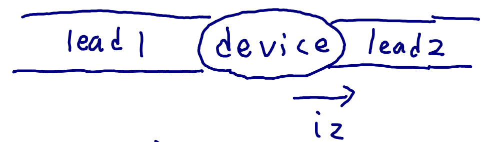
Because of conservation of probability density, we have

$$\sum_k i_k = 0 \quad \cdots\cdots (21)$$

From the condition of Eq. (21) for the steady state, we obtain

$$i_2 = -i_1 \qquad \text{-----} \ (22)$$

So, the current from the lead 1 to the lead 2 can be calculated from i_2.



$$i_{1\to2} = i_2 = -\frac{ie}{\hbar}\left(\langle\psi_2|\tau_2|\psi_d\rangle - \langle\psi_d|\tau_2^{\dagger}|\psi_2\rangle\right) \qquad \text{----} \ (23)$$

Using Eq. (13), one can calculate as

$$i_{1\to2} = -\frac{ie}{\hbar}\left(\langle\phi_{in}|\tau_1 G_d^{\dagger}\tau_2^{\dagger} g_2^{\dagger}\tau_2 G_d \tau_1^{\dagger}|\phi_{in}\rangle - \langle\phi_{in}|\tau_1 G_d^{\dagger}\tau_2^{\dagger} g_2 \tau_2 G_d \tau_1^{\dagger}|\phi_{in}\rangle\right)$$

$$= -\frac{ie}{\hbar}\langle\phi_{in}|\tau_1 G_d^{\dagger}\tau_2^{\dagger}\left(g_2^{\dagger} - g_2\right)\tau_2 G_d \tau_1^{\dagger}|\phi_{in}\rangle \qquad \text{----} \ (24)$$

By defining

$$\Gamma_2 = -i\,\tau_2^{\dagger}\left(g_2^{\dagger} - g_2\right)\tau_2 \qquad \text{-----} \ (25)$$

Eq. (24) can be rewritten as

$$i_{1\to2} = \frac{e}{\hbar}\langle\phi_{in}|\tau_1 G_d^{\dagger}\Gamma_2 G_d \tau_1^{\dagger}|\phi_{in}\rangle \qquad \text{------} \ (26)$$

☆ Equivalence of Eqs. (15) and (25).

Noting $\quad g_k(E) = \sum_n \dfrac{|\phi_{kn}\rangle\langle\phi_{kn}|}{E - E_n} \qquad \text{------} \ (27)$

$$g_k(E) - g_k^{\dagger}(E) = \sum_n |\phi_{kn}\rangle\langle\phi_{kn}|\left(\frac{1}{E-E_n+i\eta} - \frac{1}{E-E_n-i\eta}\right)$$

$$= \sum_n |\phi_{kn}\rangle\langle\phi_{kn}|\left(\frac{-2i\eta}{(E-E_n)^2+\eta^2}\right) \overset{\eta\to0}{=} \sum_n |\phi_{kn}\rangle\langle\phi_{kn}|\left(-2i\pi\,\delta(E-E_n)\right)$$

So, one can calculate as

$$\Gamma_k = -i\,\tau_k^{\dagger}\left(g_k^{\dagger} - g_k\right)\tau_k = \tau_k^{\dagger}\left(\sum_n 2\pi\,\delta(E-E_n)\,|\phi_{kn}\rangle\langle\phi_{kn}|\right)\tau_k$$

Thus, we see the definion of Eq. (25) is equivalent to Eq (15).

Now we consider all the contributions from the incident wave ϕ_{in} to the current.

Eq. 26)

$$I_{1\to 2} = 2\,\frac{e}{\hbar}\int_{-\infty}^{\infty} dE\, f(E,\mu_1)\sum_n \delta(E-E_n)\langle \phi_{in}|\tau_1 G_d^{\dagger}\Gamma_2 G_d \tau_1^{\dagger}|\phi_{in}\rangle$$

spin multiplicity

Idendity operator in the device region

$$= \frac{2e}{\hbar}\int_{-\infty}^{\infty} dE\, f(E,\mu_1)\sum_n\sum_m \delta(E-E_n)\langle \phi_{in}|\tau_1|m\rangle\langle m|G_d^{\dagger}\Gamma_2 G_d \tau_1^{\dagger}|\phi_{in}\rangle$$

$$= \frac{2e}{\hbar}\int_{-\infty}^{\infty} dE\, f(E,\mu_1)\sum_m \langle m|G_d^{\dagger}\Gamma_2 G_d \tau_1^{\dagger}\left(\sum_n \delta(E-E_n)|\phi_{in}\rangle\langle\phi_{in}|\right)\tau_1|m\rangle$$

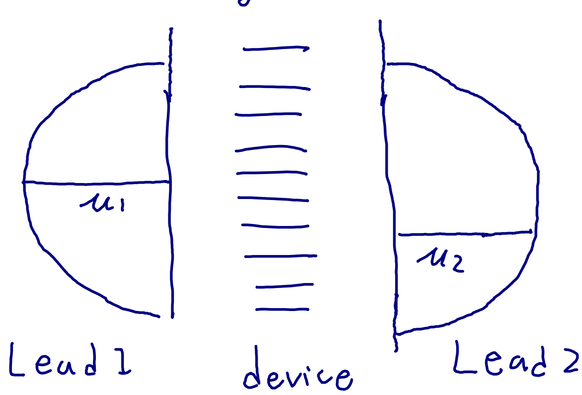
See Eq. (14)

$$= \frac{2e}{\hbar}\int_{-\infty}^{\infty} dE\, f(E,\mu_1)\sum_m \langle m|G_d^{\dagger}\Gamma_2 G_d \tau_1^{\dagger}\underbrace{\frac{a_1}{2\pi}\tau_1}_{\text{Eq.}(15)}|m\rangle$$

$$= \frac{e}{\pi\hbar}\int_{-\infty}^{\infty} dE\, f(E,\mu_1)\,\mathrm{Tr}\left(G_d^{\dagger}\Gamma_2 G_d\Gamma_1\right) \quad \cdots\cdots \quad (28)$$

$\to \frac{2e}{h}$

By considering the following situation:



Transmission

$$T(E) = \mathrm{Tr}\left(G_d^{\dagger}\Gamma_2 G_d\Gamma_1\right) \quad \cdots\cdots (30)$$

The expressions of Eqs. (29) and (30) are called <u>Landauer formura</u>

it is found that $I_{1\to 2}$ is regarded the current from the lead 1 to the lead 2. As well we need to take account of the current from the lead 2 to lead 1.

Since we assume the steady state of Eq. (22), we have the total current as

$$\boxed{I = \frac{2e}{h}\int_{-\infty}^{\infty} dE\left(f(E,\mu_1) - f(E,\mu_2)\right)\mathrm{Tr}\left(G_d^{\dagger}\Gamma_2 G_d\Gamma_1\right) \quad \cdots\cdots (29)}$$

Evaluation of G_d

The Green's function G_d of the device region is evaluated by Eq. (7). By definition, we have

$$\begin{pmatrix} E-H_1 & -\tau_1 & 0 \\ -\tau_1^\dagger & E-H_d & -\tau_2^\dagger \\ 0 & -\tau_2 & E-H_2 \end{pmatrix} \begin{pmatrix} G_1 & G_{1d} & G_{12} \\ G_{d1} & G_d & G_{d2} \\ G_{21} & G_{2d} & G_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \cdots (31)$$

row 1 × column 2

$$(E-H_1)G_{1d} - \tau_1 G_d = 0 \quad \cdots\cdots (32)$$

row 2 × column 2

$$-\tau_1^\dagger G_{1d} + (E-H_d)G_d - \tau_2^\dagger G_{2d} = 1 \quad \cdots\cdots (33)$$

row 3 × column 2

$$-\tau_2 G_d + (E-H_2)G_{2d} = 0 \quad \cdots\cdots (34)$$

From (32), we have

$$G_{1d} = (E-H_1)^{-1}\tau_1 G_d = g_1 \tau_1 G_d \quad \cdots\cdots (35)$$

From (34), we have

$$G_{2d} = (E-H_2)^{-1}\tau_2 G_d = g_2 \tau_2 G_d \quad \cdots (36)$$

Inserting Eqs. (35) and (36) into Eq. (33), we obtain

$$-\tau_1^\dagger g_1 \tau_1 G_d + (E-H_d)G_d - \tau_2^\dagger g_2 \tau_2 G_d = 1$$

$$(E-H_d-\Sigma_1-\Sigma_2)G_d = 1$$

$$G_d = (E-H_d-\Sigma_1-\Sigma_2)^{-1} \quad \cdots\cdots (37)$$

where

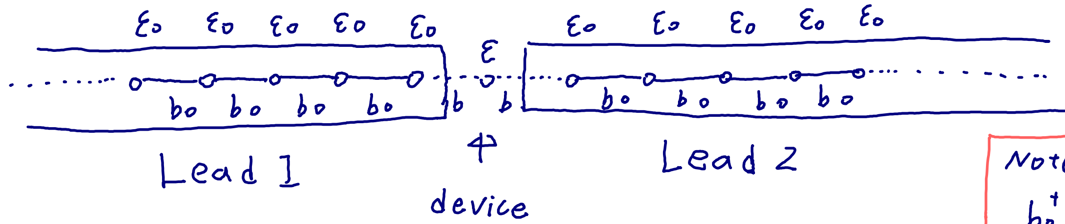
$$\Sigma_1 = \tau_1^\dagger g_1 \tau_1 \quad \cdots\cdots (38)$$

$$\Sigma_2 = \tau_2^\dagger g_2 \tau_2 \quad \cdots\cdots (39)$$

g_1 and g_2 are called surface Green's function.
Σ_1 and Σ_2 are called self-energy.

An example : linear chain model

Let's consider a linear chain model as shown below.



Note
$b_0^\dagger = b_0$

To calculate the surface Green functions of the leads 1 and 2, we employ the recursion method discussed in "Recursion_method.pdf".

From the page 13 in the lecture notes, we have

$$g_1(z) = g_2(z) = \frac{z-\varepsilon_0 - \sqrt{(z-\varepsilon_0)^2 - 4b_0^2}}{2b_0^2} \quad \cdots\cdots (40)$$

The self-energies of Eqs. (38) and (39) are given by

$$\Sigma_1(z) = \Sigma_2(z) = b^2 g_1(z) = \frac{b^2}{2b_0^2}\left(z-\varepsilon_0-\sqrt{(z-\varepsilon_0)^2-4b_0^2}\right) \quad \cdots\cdots (41)$$

The Green function of Eq. (37) is found to be

$$G_d(z) = \left[z - \varepsilon - \frac{b^2}{b_0^2}\left(z-\varepsilon_0-\sqrt{(z-\varepsilon_0)^2-4b_0^2}\right)\right]^{-1} \quad \cdots\cdots (42)$$

Also, Γ_1 and Γ_2 are calculated as

$$\Gamma_1 = \Gamma_2 = i b (g_1 - g_1^\dagger) b = \frac{i b^2}{2b_0^2}\left(z - \cancel{\varepsilon_0} - \sqrt{(z-\varepsilon_0)^2-4b_0^2} - z^* + \cancel{\varepsilon_0} + \sqrt{(z^*-\varepsilon_0)^2-4b_0^2}\right) \quad \cdots\cdots (43)$$

Thus, the transmission is given by

$$T(E) = \mathrm{Tr}\left(G_d^\dagger \Gamma_2 G_d \Gamma_1\right) \quad \cdots\cdots (44)$$

(42) (43) (42) (43)

In case that $\varepsilon = \varepsilon_0$ and $h = h_0$, we have

$$G_d(z) = \frac{1}{\sqrt{(z-\varepsilon_0)^2 - 4b^2}} \quad \cdots\cdots (45)$$

This is equivalent to Eq. (28) in the page 16 of lecture notes 2.

Taking $z = E + i\eta$ $(\eta \to 0)$, G_d becomes

$$G_d(E+i\eta) = \frac{1}{\sqrt{(E-E_0)^2 - \eta^2 + 2i\eta(E-E_0) - 4b_0^2}}$$

For $(E-E_0)^2 - 4b_0^2 < 0 \to \varepsilon_0 - 2|b_0| < E < \varepsilon_0 + 2|b_0|$

$$\mathrm{Im}\, G_d = -\frac{1}{\sqrt{4b_0^2 - (E-E_0)^2}}, \quad \mathrm{Re}\, G_d = 0 \quad \cdots\cdots (46)$$

For $E < \varepsilon_0 - 2|b_0|$, $\varepsilon_0 + 2|b_0| < E$

$$\mathrm{Im}\, G_d = 0, \quad \mathrm{Re}\, G_d = \frac{1}{\sqrt{(E-E_0)^2 - 4b_0^2}} \quad \cdots (47)$$

Noting for $\eta \to 0$

$$\Gamma_1 = \Gamma_2 = i b^2 (g_1 - g_1^+) = -2b^2 \mathrm{Im}\, g_1 = \begin{cases} \sqrt{4b_0^2 - (E-\varepsilon_0)^2} & \varepsilon_0 - 2|b_0| < E < \varepsilon_0 + 2|b_0| \\ 0 & \text{else} \end{cases} \quad \cdots\cdots (48)$$

From Eqs. (46) - (48), we obtain the transmission.

$$T(E) = \mathrm{Tr}\left(G_d^+ \Gamma_2 G_d \Gamma_1\right)$$

$$= (-i) \times i \left(\frac{1}{\sqrt{4b_0^2 - (E-\varepsilon_0)^2}}\right)^2 \times \left(\sqrt{4b_0^2 - (E-\varepsilon_0)^2}\right)^2 = 1$$

for $\varepsilon_0 - 2|b_0| < E < \varepsilon_0 + 2|b_0|$

Otherwise $\quad \cdots\cdots (49)$

$$T(E) = 0$$

Conductance quantum

Let us start Eq. (29).

$$I = \frac{2e}{h} \int_{-\infty}^{\infty} dE \; T(E) \left[f(E-\mu_1) - f(E-\mu_2) \right] \quad \cdots\cdots (29)$$

Our purpose here is to find a relation

$$I = \frac{V}{R} = VG \quad \cdots\cdots (50)$$

where V is the source-drain bias voltage, R registance, and $G \equiv \frac{1}{R}$ conductance. To derive Eq. (50) based on Eq. (29), we consider a case that $\mu_1 = \mu_2 + eV = \mu + eV$ with a tiny V.

Then, Eq. (29) can be approximated by

$$I \simeq \frac{2e}{h} \int_{-\infty}^{\infty} dE \left[T(\mu) + \left. \frac{\partial T(E)}{\partial E} \right|_{E=\mu} (E-\mu) \right] \left[f(E-\mu) + \left. \frac{\partial f(E-(\mu+eV))}{\partial V} \right|_{V=0} V - f(E-\mu) \right]$$

$$= \frac{2e}{h} \left[\int_{-\infty}^{\infty} dE \; T(\mu) \frac{\partial f(E-(\mu+eV))}{\partial V} V + \int_{-\infty}^{\infty} dE \frac{\partial T(E)}{\partial E} (E-\mu) \frac{\partial f(E-(\mu+eV))}{\partial V} V \right] \quad \cdots\cdots (51)$$

Noting $\frac{\partial f(E-(\mu+eV))}{\partial V} = -e \frac{\partial f(E-(\mu+eV))}{\partial E} \xrightarrow{V \to 0} e\,\delta(E-\mu)$

Eq. (51) becomes

$$I = \frac{2e^2}{h} T(\mu) V \int_{-\infty}^{\infty} dE \; \delta(E-\mu) = V \left(T(\mu) \frac{2e^2}{h} \right) \quad \cdots\cdots (52)$$

Compared to Eq. (50), we obatin

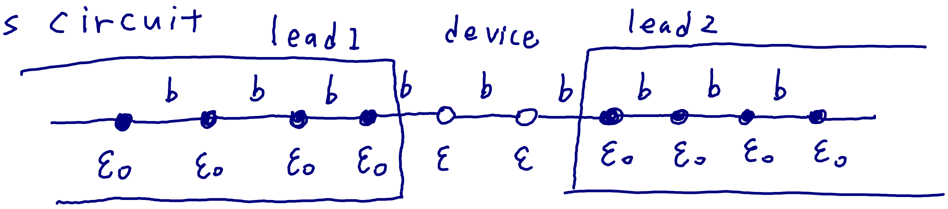
$$G = T(\mu)\, G_0 \quad \cdots\cdots (53)$$

$$G_0 = \frac{2e^2}{h} \quad \cdots\cdots (54)$$

G_0 is called conductance quantum

Conductance of series and parallel circuits

(a) series circuit



$\varepsilon_0 = 0$

As well as the lecture notes 2 and 13, the surface Green functions are given by

$$g_1(z) = g_2(z) = \frac{z - \sqrt{z^2 - 4b^2}}{2b^2} \quad \cdots\cdots (1)$$

The self-energies can be calculated as

$$\Sigma_1(z) = \begin{pmatrix} b \\ 0 \end{pmatrix} g_1(z) \,(b,\ 0) = \begin{pmatrix} b^2 g_1(z) & 0 \\ 0 & 0 \end{pmatrix} \quad \cdots\cdots (2)$$

$$\Sigma_2(z) = \begin{pmatrix} 0 \\ b \end{pmatrix} g_2(z) \,(0\ \ b) = \begin{pmatrix} 0 & 0 \\ 0 & b^2 g_2(z) \end{pmatrix} \quad \cdots\cdots (3)$$

The Green function of the device region is given by

$$G_d(z) = \left(z - H_d - \Sigma_1(z) - \Sigma_2(z) \right)^{-1}$$

$$= \begin{pmatrix} z - \varepsilon - \frac{1}{2}\left(z - \sqrt{z^2 - 4b^2}\right) & -b \\ -b & z - \varepsilon - \frac{1}{2}\left(z - \sqrt{z^2 - 4b^2}\right) \end{pmatrix}^{-1} = \begin{pmatrix} A & B \\ B & A \end{pmatrix}^{-1} = \frac{1}{A^2 - B^2} \begin{pmatrix} A & -B \\ -B & A \end{pmatrix}$$

$$= \frac{1}{C} \begin{pmatrix} z - \varepsilon - \frac{1}{2}\left(z - \sqrt{z^2 - 4b^2}\right) & b \\ b & z - \varepsilon - \frac{1}{2}\left(z - \sqrt{b^2 - 4b^2}\right) \end{pmatrix}$$

$$= \begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix} \quad \cdots\cdots (4)$$

$$C = \left[z - \varepsilon - \frac{1}{2}\left(z - \sqrt{z^2 - 4b^2}\right) \right]^2 - b^2 \quad \cdots\cdots (5)$$

Γ_1 and Γ_2 can be calculated as

$$\Gamma_1 = i\tau_1^{+}(g_1 - g_1^{+})\tau_1 = i\begin{pmatrix} b \\ 0 \end{pmatrix} 2i\,\mathrm{Im}\,g_1 \begin{pmatrix} b & 0 \end{pmatrix}$$

$$= -2b^2\,\mathrm{Im}\,g_1 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \sqrt{4b^2 - E^2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\Gamma_2 = i\tau_2^{+}(g_2 - g_2^{+})\tau_1 = i\begin{pmatrix} 0 \\ b \end{pmatrix} 2i\,\mathrm{Im}\,g_2 \begin{pmatrix} 0 & b \end{pmatrix}$$

$$= -2b^2\,\mathrm{Im}\,g_2 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \sqrt{4b^2 - E^2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\text{for} \quad -2|b| < E < 2|b| \qquad \cdots\cdots (6)$$

otherwise, they are zero.

Then, one can calculate the transmission as

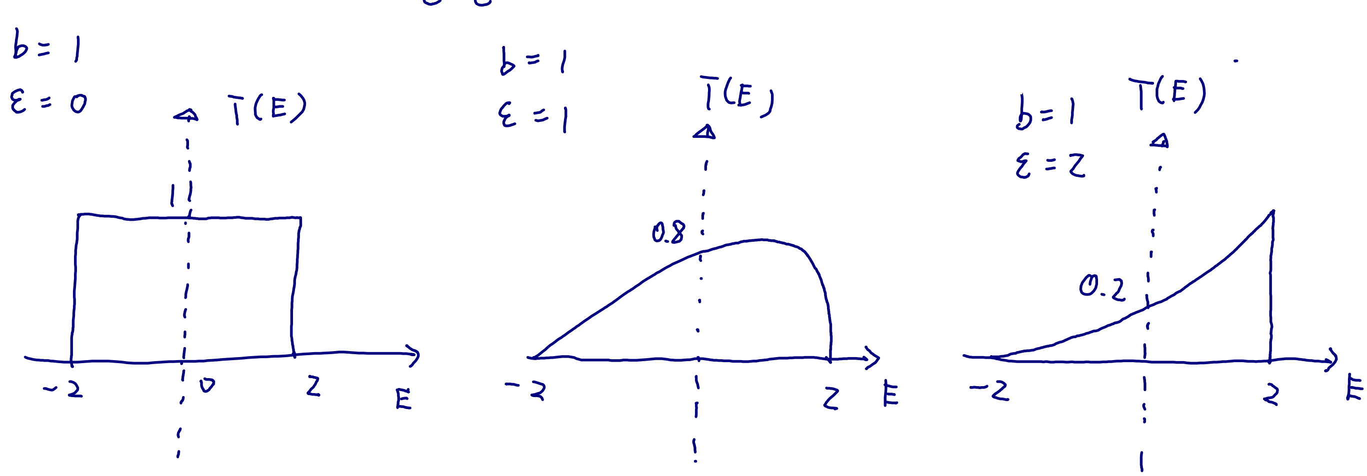
$$T(E) = \mathrm{Tr}\left(G_d^{\dagger}\Gamma_2 G_d \Gamma_1\right)$$

$$= (4b^2 - E^2)\,\mathrm{Tr}\left[\begin{pmatrix} \alpha^* & \beta^* \\ \beta^* & \alpha^* \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\right]$$

$$= (4b^2 - E^2)\,\mathrm{Tr}\left[\begin{pmatrix} 0 & \beta^* \\ 0 & \alpha^* \end{pmatrix}\begin{pmatrix} \alpha & 0 \\ \beta & 0 \end{pmatrix}\right] = (4b^2 - E^2)\,\mathrm{Tr}\begin{pmatrix} \beta^*\beta & 0 \\ \alpha^*\beta & 0 \end{pmatrix}$$

$$= (4b^2 - E^2)\,\beta^*\beta$$

$$= (4b^2 - E^2) \times b^2 \times \frac{1}{c^* c} \qquad \cdots\cdots (7)$$



Noting that $T(E)$ at $E=0$ is the conductance,

we have c^*c at $E=0$ as

$$c^*c\,(E=0) = \left[(-\varepsilon+ib)^2-b^2\right]\left[(-\varepsilon-ib)^2-b^2\right]$$

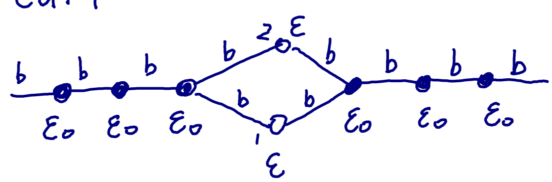
$$= 4b^4+\varepsilon^4 \qquad \text{----}\ (8)$$

Thus, we obtain from Eqs. (7) and (8)

$$G = 4b^2 \times b^2 \times \frac{1}{c^*c\,(E=0)}$$

$$= \frac{4b^4}{4b^4+\varepsilon^4} \quad \text{in } G_0 \qquad \text{-----}\ (9)$$

(b) Parallel circuit



The surface Green functions are given by Eqs. (1).

The self-energies can be calculated as

$$\Sigma_1(z) = \begin{pmatrix} b \\ b \end{pmatrix} g_1(z)\begin{pmatrix} b & b \end{pmatrix} = b^2 g_1(z)\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \qquad \text{-----}\ (10)$$

$$\Sigma_2(z) = \begin{pmatrix} b \\ b \end{pmatrix} g_2(z)\begin{pmatrix} b & b \end{pmatrix} = b^2 g_2(z)\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \qquad \text{-----}\ (11)$$

The Green function of the device region is given by

$$G_d(z) = (zI - H_d - \Sigma_1 - \Sigma_2)^{-1}$$

$$= \begin{pmatrix} \cancel{z}-\varepsilon-\cancel{z}+\sqrt{z^2-4b^2} & -z+\sqrt{z^2-4b^2} \\ -z+\sqrt{z^2-4b^2} & \cancel{z}-\varepsilon-\cancel{z}+\sqrt{z^2-4b^2} \end{pmatrix}^{-1} = \begin{pmatrix} A & B \\ B & A \end{pmatrix}^{-1} = \frac{1}{A^2-B^2}\begin{pmatrix} A & -B \\ -B & A \end{pmatrix}$$

$$\text{-----}\ (12)$$

$$G_d(z) = \frac{1}{c}\begin{pmatrix} -\varepsilon + \sqrt{z^2-4b^2} & z - \sqrt{z^2-4b^2} \\ z - \sqrt{z^2-4b^2} & -\varepsilon + \sqrt{z^2-4b^2} \end{pmatrix} \quad \cdots\cdots (13)$$

$$c = \left(-\varepsilon + \sqrt{z^2-4b^2}\right)^2 - \left(z - \sqrt{z^2-4b^2}\right)^2 \quad \cdots\cdots (14)$$

Γ_1 and Γ_2 can be calculated as

$$\Gamma_1 = i\tau_1^\dagger (g_1 - g_1^\dagger)\tau_1$$

$$= i\begin{pmatrix} b \\ b \end{pmatrix} 2i\,\mathrm{Im}\, g_1 \begin{pmatrix} b & b \end{pmatrix} = -2b^2\,\mathrm{Im}\, g_1 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$= \sqrt{4b^2-E^2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad \cdots\cdots (15)$$

$$\Gamma_2 = i\tau_2^\dagger (g_2 - g_2^\dagger)\tau_2 = -2b^2\,\mathrm{Im}\, g_2 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$= \sqrt{4b^2-E^2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad \cdots\cdots (16)$$

for $-2|b| < E < 2|b|$

otherwise, they are zero.

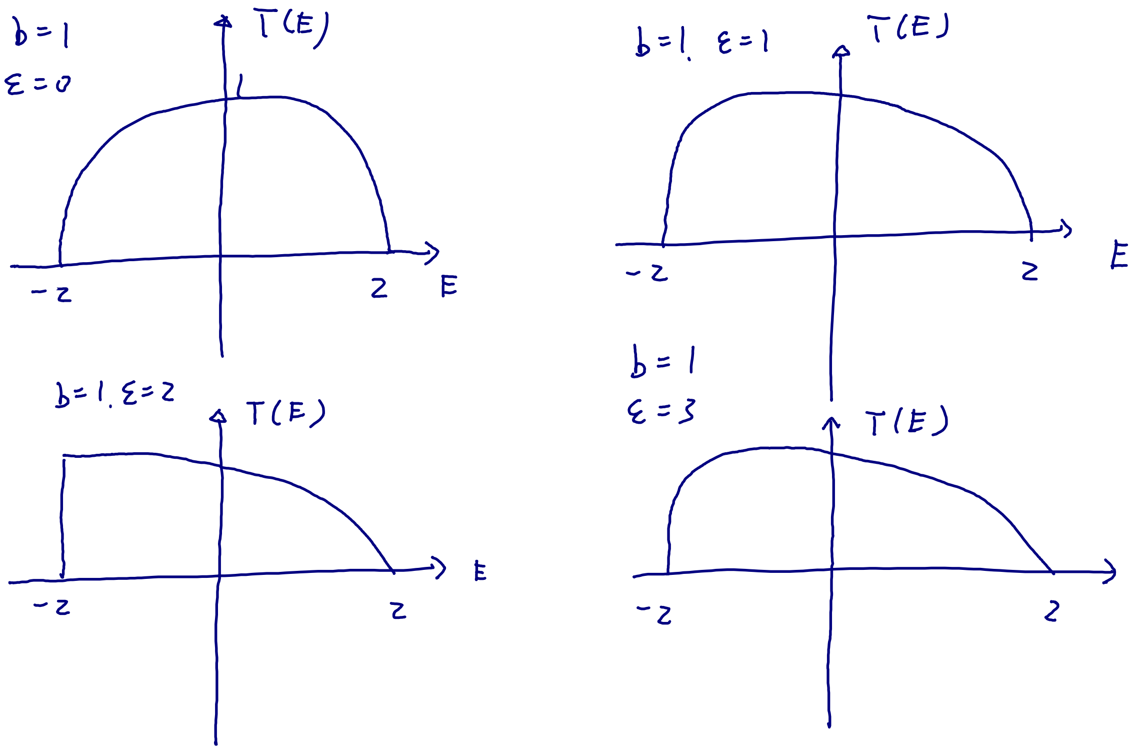
So, the transmission are given by

$$T(E) = \mathrm{Tr}\left(G_d^\dagger \Gamma_2 G_d \Gamma_1\right)$$

$$= \frac{1}{c^* c}(4b^2-E^2)\,\mathrm{Tr}\left[\begin{pmatrix} -\varepsilon + \sqrt{z^{*2}-4b^2} & z^* - \sqrt{z^{*2}-4b^2} \\ z^* - \sqrt{z^{*2}-4b^2} & -\varepsilon + \sqrt{z^{*2}-4b^2} \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\right.$$

$$\left.\times \begin{pmatrix} -\varepsilon + \sqrt{z^2-4b^2} & z - \sqrt{z^2-4b^2} \\ z - \sqrt{z^2-4b^2} & -\varepsilon + \sqrt{z^2-4b^2} \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\right]$$

$$T(E) = \frac{-4E^2 + 16b^2}{\left(\varepsilon + z - 2\sqrt{z^2 - 4b^2}\right)\left(\varepsilon + z^* - 2\sqrt{z^{*2} - 4b^2}\right)} \quad \cdots\cdots (17)$$



From Eq. (17) at $E=0$, we obtain the conductance

$$G = \frac{16b^2}{(\varepsilon - 2\times 2bi)(\varepsilon + 2\times 2bi)} = \frac{16b^2}{\varepsilon^2 + 16b^2} \quad \cdots (18)$$

in G_0

Conductance of 

$$\frac{4b^2}{(-\varepsilon + 2b)^2} \quad \cdots\cdots (19)$$

Comparing with Eqs. (9), (18), and (19), we see that Ohm' law is not valid any more.