Notes on quantum transport in mesoscopic systems

Li Gaoyang
(Dated: 2020/12/1)

I. NONEQUILIBRIUM GREEN'S FUNCTION TECHNIQUE

A. Demonstrative Hamiltonian

$$\hat{H} = H_{lead} + H_{dot} + H_T \tag{1}$$

$$H_{lead} = \sum_{k\alpha} \epsilon_{k\alpha} \hat{C}^{\dagger}_{k\alpha} \hat{C}_{k\alpha} \tag{2}$$

$$\epsilon_{k\alpha} = \epsilon^{(0)}_{k\alpha} + qv_{\alpha} \tag{3}$$

$$H_{dot} = \sum_n (\epsilon_n + qU_n)\, d^{\dagger}_n d_n \tag{4}$$

$$U_n = \sum_m V_{nm} < d^{\dagger}_m d_m > \tag{5}$$

$$H_T = \sum_{k\alpha n} \left[t_{k\alpha n} \hat{C}^{\dagger}_{k\alpha} \hat{d}_n + t^*_{k\alpha n} \hat{d}^{\dagger}_n \hat{C}_{k\alpha} \right] \tag{6}$$

B. Current definition

We use the Hamiltonian in WangJian's notes. Equation of motion of particle operator $\hat{N}_{\alpha k\sigma}$ in the lead α is

$$\begin{aligned}
\frac{d}{dt}\hat{N}_{\alpha} = \frac{i}{\hbar}[H, \sum_k c^{\dagger}_{\alpha k} c_{\alpha k}] &= \left[\sum_{k'n,\alpha'=L,R} \left[t_{k'\alpha'} c^{\dagger}_{k'\alpha'} d_n + \text{c.c.} \right], \sum_k c^{\dagger}_{\alpha k} c_{\alpha k} \right] \\
&= \frac{i}{\hbar} \sum_{kk',n,\alpha'=L,R} \left[-t_{k'\alpha'} c^{\dagger}_{k'\alpha'} d_n \delta_{\alpha\alpha'} \delta_{kk'} + \text{c.c.} \right] \\
&= \frac{i}{\hbar} \sum_{kn} [-t_{k\alpha} c^{\dagger}_{k\alpha} d_n + t^*_{k\alpha} d^{\dagger}_n c_{k\alpha}]
\end{aligned} \tag{7}$$

So, the charge current is given by

$$\begin{aligned}
I_{\alpha}(t) &= e\langle \frac{d}{dt}\hat{N}_{\alpha}(t) \rangle \\
&= \frac{ie}{\hbar} \sum_{kn} (\langle -t_{k\alpha} c^{\dagger}_{k\alpha}(t) d_n(t) \rangle + \langle t^*_{k\alpha} d^{\dagger}_n(t) c_{k\alpha}(t) \rangle)
\end{aligned} \tag{8}$$

Define the lesser Green's function

$$G^{<}_{\sigma',k\alpha\sigma}(t,t') = i\langle c^{\dagger}_{k\alpha\sigma}(t') d_{\sigma'}(t) \rangle \tag{9}$$

the charge current is written as

$$I_L(t) = \frac{-e}{\hbar} \sum_{kn\alpha \in L} (t_{k\alpha n} G^{<}_{n,k\alpha\sigma}(t,t) - t^*_{k\alpha n} G_{k\alpha,n}(t,t)\rangle) \tag{10}$$

More generally, we define the contour Green's function

$$G_{n,k\alpha}(\tau,\tau') = -i\langle d_n(\tau) c^\dagger_{k\alpha}(\tau')\rangle. \tag{11}$$

Following Jauho's notation [2], when the electron in the lead is non-interacting, $\mathrm{G}_{n,k\alpha\sigma}(\tau,\tau')$ is related to G_{nm} and $g_{k\alpha}$ by the following contour integral

$$G_{n,k\alpha}(\tau,\tau') = \sum_m \int d\tau_1 G_{nm}(\tau,\tau_1)\, t^*_{k\alpha m} g_{k\alpha}(\tau_1,\tau') \tag{12}$$

where

$$G_{nm}(\tau_1,\tau_2) \equiv -i\langle T_c\left[d_n(\tau_1)\, d^\dagger_m(\tau_2)\right]\rangle \tag{13}$$

$$g_{k\alpha}(\tau_1,\tau_2) \equiv -i\langle T_c\left[c_{k\alpha}(\tau_1)\, c^\dagger_{k\alpha}(\tau_2)\right]\rangle_0. \tag{14}$$

Using the theorem of analytic continuation, we have

$$\begin{aligned} G^{<}_{n,k\alpha}(t,t') = \sum_m \int dt_1 \left[G^r_{nm}(t,t_1)\, t^*_{k\alpha m} g^{<}_{k\alpha}(t_1,t')\right. \\ \left. + G^{<}_{nm}(t,t_1)\, t^*_{k\alpha m} g^a_{k\alpha}(t_1,t')\right]. \end{aligned} \tag{15}$$

This gives the term in current

$$\begin{aligned} &\textstyle\sum_{kn} t_{k\alpha n} G^{<}_{n,k\alpha}(t,t') = \sum_{kmn} \int dt_1 t_{k\alpha n} t^*_{k\alpha m} \\ &\times \left[G^r_{nm}(t,t_1)\, g^{<}_{k\alpha}(t_1,t') + G^{<}_{nm}(t,t_1)\, g^a_{k\alpha}(t_1,t')\right] \\ &= \textstyle\sum_n \int dt_1 \left[G^r(t,t_1)\, \Sigma^{<}_\alpha(t_1,t') + G^{<}(t,t_1)\, \Sigma^a_\alpha(t_1,t')\right]_{nn} \end{aligned} \tag{16}$$

matrix element of the self-energy Σ_α due to lead α is

$$\Sigma^\gamma_{\alpha,mn}(t_1,t_2) = \sum_k t^*_{k\alpha m}(t_1) g^\gamma_{k\alpha}(t_1,t_2) t_{k\alpha n}(t_2). \tag{17}$$

Here, the matrix index are m, n, which is index for energy level of central scattering area. Substitute **??** in charge current, we have

$$\begin{aligned} I_\alpha(t) = -\frac{e}{\hbar} \int dt_1 \operatorname{Tr}\left[G^r(t,t_1)\, \Sigma^{<}_\alpha(t_1,t)\right. \\ \left. + G^{<}(t,t_1)\, \Sigma^a_\alpha(t_1,t)\right] + h.c. \end{aligned} \tag{18}$$

where the summation over index n is abbreviated in to matrix summation notation Tr, and summation index k goes into self-energy matrix Σ_α.

C. Free propagators

Here we assume a time-dependent external voltage v_α. The free Green's functions of lead electrons are (XXX)

$$g^{<}_{k\sigma}(t,t') \equiv i\left\langle c^\dagger_{k\sigma}(t')\, c_{k\sigma}(t)\right\rangle = if(\varepsilon^{(0)}_k) e^{-i\int_{t'}^{t} dt_1 \varepsilon_{k\sigma}(t_1)} \tag{19}$$

$$g^{>}_{k\sigma}(t,t') \equiv -i\left\langle c_{k\sigma}(t) c^\dagger_{k\sigma}(t')\right\rangle = i\left[f(\varepsilon_k) - 1\right] e^{-i\varepsilon_{k\sigma}(t-t')} \tag{20}$$

$$g^r_{k\sigma}(t) \equiv -i\theta(t)\left\langle\left[c_{k\sigma}(t), c^\dagger_{k\sigma}(t')\right]_+\right\rangle = -i\theta(t)e^{-i\varepsilon_{k\sigma}(t-t')} \tag{21}$$

$$g^a_{k\sigma}(t) \equiv i\theta(-t)\left\langle\left[c_{k\sigma}(t), c^\dagger_{k\sigma}(t')\right]_+\right\rangle = i\theta(-t)e^{-i\varepsilon_{k\sigma}(t-t')} \tag{22}$$

Using the relation

$$\int dte^{i\omega t} = 2\pi\delta(\omega), \tag{23}$$

Fourier transformation gives

$$g^<_{k\sigma}(\omega) = 2\pi i f(\varepsilon_{k\sigma})\,\delta(\omega-\varepsilon_{k\sigma}) = if(\varepsilon_{k\sigma})\,A_0(k,\omega) \tag{24}$$

$$g^>_{k\sigma}(\omega) = 2\pi i\left[f(\varepsilon_{k\sigma})-1\right]\delta(\omega-\varepsilon_{k\sigma}) \tag{25}$$

$$g^r_{k\sigma}(\omega) = -i\int_{-\infty}^{\infty} dte^{i\omega t}\theta(t)e^{-i\epsilon_{k\sigma}t} = -i\int_0^\infty dte^{i(\omega-\epsilon_{k\sigma})t} = \frac{-i}{i(\omega-\varepsilon_{k\sigma})}e^{i(\omega-\varepsilon)}|_0^{+\infty} \tag{26}$$

To make the integral converge at the upper limit, we let $\omega \to \omega + i0^+$, where 0^+ is a positive infinitesimal, which yields

$$g^r_{k\sigma}(\omega) = \frac{1}{\omega-\varepsilon_{k\sigma}+i0^+}. \tag{27}$$

Similarly,

$$g^a_{k\sigma}(\omega) = \frac{1}{\omega-\varepsilon_{k\sigma}-i0^+}. \tag{28}$$

Then we have

$$g^r_{k\sigma}(\omega) - g^a_{k\sigma}(\omega) = -2\pi i\delta(\omega-\varepsilon_{k\sigma}) \tag{29}$$

The fermion spectral function is defined as

$$\begin{aligned} A_0(k\sigma,\omega) &= i\left[g^r_{k\sigma}(\omega) - g^a_{k\sigma}(\omega)\right] \\ &= -2\Im\mathrm{m}\left[g^r_{k\sigma}(\omega)\right] \\ &= 2\pi\delta(\omega-\varepsilon_{k\sigma}) \end{aligned} \tag{30}$$

where the following relation are used

$$\frac{1}{x\pm i\eta} = \mathcal{P}\frac{1}{x} \mp i\pi\delta(x), \quad \eta = 0^+, \tag{31}$$

$$\Im\mathrm{m}\left[g^r_{k\sigma}(\omega)\right] = -\pi\delta(\omega-\varepsilon_k). \tag{32}$$

D. DC case

$$G^\gamma(t,t_1) = G^\gamma(t-t_1) \tag{33}$$

and

$$\Sigma^\gamma(t,t_1) = \Sigma^\gamma(t-t_1) \tag{34}$$

where

$$\gamma = <, >, r, a. \tag{35}$$

Recall that

$$\left[G^{<}\right]^{\dagger}(E) = -G^{<}(E) \tag{36}$$

$$\left[G^{r}\right]^{\dagger} = G^{a} \tag{37}$$

and using equation (221) in WangJian's note, we have charge current for DC bias

$$\begin{aligned} I_{\alpha} = -\frac{e}{\hbar}\int \frac{dE}{2\pi}\,\mathrm{Tr}\left[\left(G^{r}(E) - G^{a}(E)\right)\Sigma_{\alpha}^{<}(E)\right. \\ \left. +G^{<}(E)\left(\Sigma_{\alpha}^{a}(E) - \Sigma_{\alpha}^{r}(E)\right)\right] \end{aligned} \tag{38}$$

Substitute free propagators in, we have

$$\Sigma_{\alpha,mn}^{<}(t-t_1) = \sum_k t_{k\alpha m}^{*}(t_1) g_{k\alpha}^{<}(t_1-t_2) t_{k\alpha n}(t_2) = i\sum_k t_{k\alpha m}^{*}(t_1) f(\epsilon_{k\alpha}) e^{-i\varepsilon_{k\alpha(t-t_1)}} t_{k\alpha n}(t_2) \tag{39}$$

Fourier transformation gives (dependent variable $\epsilon_{k\alpha}$ not ω?, check Eq.(71) in WangJ's note Chap2?)

$$\Sigma_{\alpha,mn}^{<}(E) = 2\pi i \sum_k t_{k\alpha m}^{*} f(\varepsilon_{k\alpha}) t_{k\alpha n}\delta(E-\varepsilon_{k\alpha}) \tag{40}$$

$$\Sigma_{\alpha}^{a}(E) - \Sigma_{\alpha}^{r}(E) = \sum_k t_{k\alpha m}^{*}(g_{k\alpha}^{a}(E) - g_{k\alpha}^{r}(E)) t_{k\alpha n} \tag{41}$$

which according to Eq. (29), we have

$$\Sigma_{\alpha}^{a}(E) - \Sigma_{\alpha}^{r}(E) = 2\pi i\sum_k t_{k\alpha m}^{*}\delta(E-\epsilon_{k\alpha}) t_{k\alpha n}. \tag{42}$$

Define a level-width function:

$$\Gamma_{\alpha,mn}(E) = \sum_k 2\pi t_{k\alpha m}^{*} t_{k\alpha n}\delta\left(E-\varepsilon_{k\alpha}\right) \tag{43}$$

So it gives equations(the fermion distribution is factorized out of summation k?)

$$\Sigma_{\alpha,mn}^{<}(E) = i f(\varepsilon_{k\alpha})\Gamma_{\alpha,mn}(E) \tag{44}$$

and

$$\Sigma_{\alpha}^{a}(E) - \Sigma_{\alpha}^{r}(E) = i\Gamma_{\alpha,mn}(E) \tag{45}$$

Then Eq. (38) can be written as

$$\begin{aligned} I_{\alpha} =& -\frac{e}{\hbar}\int\frac{dE}{2\pi}\,\mathrm{Tr}[\left(G^{r}(E) - G^{a}(E)\right)\left(if(\varepsilon_{k\alpha}\Gamma_{\alpha,mn}(E))\right) \\ &+ G^{<}(E)(i\Gamma_{\alpha,mn}(E))] \\ =& -\frac{ie}{\hbar}\int\frac{dE}{2\pi}\,\mathrm{Tr}\left[\Gamma_{\alpha,mn}(E)(\left[G^{r}(E) - G^{a}(E)\right] f(\varepsilon_{k\alpha}) + G^{<}(E))\right] \end{aligned} \tag{46}$$

In steady state, $I = I_L = -I_R$, or $I = I_L + I_R = (I_L - I_R)/2$, this leads to the general expression for the dc-current

$$\begin{aligned} I = -\frac{\mathrm{i}e}{2\hbar}\int\frac{\mathrm{d}\varepsilon}{2\pi}\,\mathrm{Tr}\left\{\left[\boldsymbol{\Gamma}^{L}(\varepsilon) - \boldsymbol{\Gamma}^{R}(\varepsilon)\right]\mathbf{G}^{<}(\varepsilon)\right. \\ \left. + \left[f_L(\varepsilon)\boldsymbol{\Gamma}^{L}(\varepsilon) - f_R(\varepsilon)\boldsymbol{\Gamma}^{R}(\varepsilon)\right]\left[\mathbf{G}^{\mathrm{r}}(\varepsilon) - \mathbf{G}^{\mathrm{a}}(\varepsilon)\right]\right\} \end{aligned} \tag{47}$$

if the left and right line-width functions are proportional to each other,

$$\mathbf{\Gamma}^L(\varepsilon) = \lambda \mathbf{\Gamma}^R(\varepsilon) \tag{48}$$

and fix the arbitrary parameter x, i.e. $x = 1/(1+\lambda)$, gives

$$\begin{aligned} J &= \frac{1e}{\hbar}\int \frac{\mathrm{d}\varepsilon}{2\pi}\left[f_L(\varepsilon) - f_R(\varepsilon)\right]\mathcal{T}(\varepsilon) \\ \mathcal{T}(\varepsilon) &= \mathrm{Tr}\left\{\frac{\Gamma^L(\varepsilon)\Gamma^R(\varepsilon)}{\Gamma^L(\varepsilon)+\Gamma^R(\varepsilon)}\left[\mathbf{G}^{\mathrm{r}}(\varepsilon) - \mathbf{G}^{\mathrm{a}}(\varepsilon)\right]\right\} \end{aligned} \tag{49}$$

Despite the apparent similarity of (12.27) to the Landauer formula, it is important to bear in mind that, in general, there is no immediate connection between the quantity $\mathcal{T}(\varepsilon)$ and the transmission coefficient $T(\varepsilon)$.

E. Another way to get $G_{n,k\alpha}(\tau,\tau')$(Dyson equation + Keldysh equation)

Denote G_0 the Green's function of the isolated quantum dot and leads corresponding to the Hamiltonian H_0, and G the Green's function of the open system corresponding to H, one has the Dyson equation

$$G = G_0 + G_0 \Sigma G \tag{50}$$

Use the theorem of analytic continuation on Dyson equation, we get the Keldysh equation (in matrix representation)

$$G^{<,>} = G_0^{<,>} + G^r\Sigma^r G_0^{<,>} + G^{<,>}\Sigma^a G_0^a + G^r\Sigma^{<,>}G_0^a \tag{51}$$

or

$$G^{<,>} = G_0^{<,>} + G_0^r\Sigma^r G^{<,>} + G_0^{<,>}\Sigma^a G^a + G_0^r\Sigma^{<,>}G^a \tag{52}$$

or

$$G^{<} = G^r\left(G_0^r\right)^{-1}G_0^{<}\left(G_0^a\right)^{-1}G^a + G^r\Sigma^{<}G^a \tag{53}$$

See Eq. (77) in WangJian's notes.

F. With spin index

The demonstrative current of lead β with spin σ is [?]

$$\begin{aligned} I_{\beta\sigma} = \tfrac{e}{\hbar}\textstyle\sum_{k,i,j}\int d\omega V_{ki\beta\sigma}V^*_{kj\beta\sigma}\Big\{&\left[G^r_{i\sigma,j\sigma}(\omega) - G^a_{i\sigma,j\sigma}(\omega)\right]g^<_{k\beta\sigma}(\omega) \\ &-\left[g^r_{k\beta\sigma}(\omega) - g^a_{k\beta\sigma}(\omega)\right]G^<_{i\sigma,j\sigma}(\omega)\Big\}. \end{aligned} \tag{54}$$

Substitute free propagators into current formula, we have

$$I_{\beta\sigma} = \frac{ie}{h}\sum_{i,j}\int d\omega\Gamma_{ij\beta\sigma}(\omega)\left\{\left[G^r_{i\sigma,j\sigma}(\omega) - G^a_{i\sigma,j\sigma}(\omega)\right]f_\beta(\omega) + G^<_{i\sigma,j\sigma}(\omega)\right\} \tag{55}$$

self-energy of lead α is

$$\Sigma^<_\alpha(\omega) = i\Gamma_\alpha\left(\omega - qv_\alpha\right)f_\alpha(\omega) \tag{56}$$

II. APPENDIX: ANALYTIC CONTINUATION

We list here all the analytic continuations used in this work. For $C = AB$ (matrix multiplication), we have[**?**]

$$C^< = A^r B^< + A^< B^a, \quad \text{and} \quad C^> = A^r B^> + A^> B^a \tag{57}$$

and

$$C^r = A^r B^r, \quad \text{and} \quad C^a = A^a B^a \tag{58}$$

For $C(\tau, \tau') = A(\tau, \tau')B(\tau, \tau')$ or $C = A.B$ (the Hadamard matrix product), we have[**?**]

$$C^< = A^<.B^<, \quad \text{and} \quad C^> = A^>.B^> \tag{59}$$

and

$$\begin{aligned} C^r &= A^r.B^< + A^<.B^r + A^r.B^r, \\ C^a &= A^a.B^< + A^<.B^a + A^a.B^a \end{aligned} \tag{60}$$

For $C(\tau, \tau') = A(\tau, \tau')B(\tau', \tau)$ or $C = A.\tilde{B}$ where $\tilde{B}(t_1, t_2) \equiv B(t_2, t_1)$, we have[**?**]

$$C^< = A^<.\tilde{B}^>, \quad \text{and} \quad C^> = A^>.\tilde{B}^< \tag{61}$$

$$\begin{aligned} C^r &= A^<.\tilde{B}^a + A^r.\tilde{B}^<, \\ C^a &= A^<.\tilde{B}^r + A^a.\tilde{B}^< \end{aligned} \tag{62}$$

For $D = ABC$, we have

$$D^< = A^r B^r C^< + A^r B^< C^a + A^< B^a C^a, \tag{63}$$

and

$$D^r = A^r B^r C^r. \tag{64}$$

From Eqs. (61) and (62), one can easily check the relation $C^> - C^< = C^r - C^a$ which must be satisfied.

[1] Y, K, Kato. Observation of the Spin Hall Effect in Semiconductors[J]. Science, 2004.
[2] Antti-Pekka Jauho, Quantum Kinetics in Transport and Optics of Semiconductors, P188.
[3] L. Gu, H. H. Fu, and R. Q. Wu, Phys. Rev. B 94, 115433 (2016).
[4] J. Ren, Phys. Rev. B 88, 220406 (2013).