NEGF Notes

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A. Hamiltonian

$$H = H_L + H_R + H_d + H_T + H_{sd} \tag{1}$$

$$H_L = \sum_{k\sigma} \epsilon_{k\sigma,L} c^\dagger_{k\sigma} c_{k\sigma} \tag{2}$$

$$H_R = \sum_q \omega_q a^\dagger_q a_q \tag{3}$$

$$H_d = \sum_{n\sigma} \epsilon_{n\sigma} d^\dagger_{n\sigma} d_{n\sigma} \tag{4}$$

$$H_T = \sum_{k\sigma n} \left(t_{k\sigma n} c^\dagger_{k\sigma} d_{n\sigma} + t^*_{k\sigma n} d^\dagger_{n\sigma} c_{k\sigma} \right) \tag{5}$$

$$H_{sd} = -\sum_{qnm} J_q \left(d^\dagger_{n\uparrow} d_{m\downarrow} a^\dagger_q + a_q d^\dagger_{m\downarrow} d_{n\uparrow} \right) \delta \left(\epsilon_{n\uparrow} - \epsilon_{m\downarrow} - \omega_q \right) \tag{6}$$

$$s^+_q = \sum_{nm} d^\dagger_{n\uparrow} d_{m\downarrow} \delta_{\uparrow\downarrow} \tag{7}$$

$$s^-_q = \sum_{nm} d^\dagger_{m\downarrow} d_{n\uparrow} \delta_{\uparrow\downarrow} \tag{8}$$

1. check operators

$$i\dot{a}_q = \omega_q a_q - J_q s^+_q \tag{9}$$

$$i\dot{c}_{k\sigma} = \epsilon_{k\sigma,L} c_{k\sigma} + \sum_{k'} t_{k\sigma n} d_{n\sigma} \tag{10}$$

$$i\dot{d}_{n\uparrow} = \epsilon_{n\uparrow} d_{n\uparrow} + \sum_k t^*_{k\uparrow n} c_{k\uparrow} - \sum_{q,m} J_q a^\dagger_q d_{m\downarrow} \delta(\epsilon_{n\uparrow} - \epsilon_{m\downarrow} - \omega_q) \tag{11}$$

$$i\dot{d}_{n\downarrow} = \epsilon_{n\downarrow} d_{n\downarrow} + \sum_k t^*_{k\downarrow n} c_{k\downarrow} - \sum_{q,m} J_q a_q d_{m\uparrow} \delta(\epsilon_{m\uparrow} - \epsilon_{n\downarrow} - \omega_q) \tag{12}$$

B. spin current ???

Define

$$G_{d,R}\left(\tau, \tau'\right) = -i \langle s^+_q(\tau) a^\dagger_q(\tau') \rangle. \tag{13}$$

The lesser Green's function is(s_q^+ is fermionic but a_q is bosonic)

$$G_{d,R}^{<}\left(t,t'\right) = -i\langle a_q^{\dagger}(t')s_q^{+}(t)\rangle \tag{14}$$

We also define the Green's function that is related to the QD (not the Green's function of the QD),

$$G_d\left(\tau,\tau'\right) = -i\left\langle T_c S s_q^{+}(\tau) s_q^{-}\left(\tau'\right)\right\rangle . \tag{15}$$

We have

$$-i\partial_{\tau'}G_{d,R}\left(\tau,\tau'\right) = \omega_q G_{d,R}\left(\tau,\tau'\right) - J_q G_d \tag{16}$$

or

$$G_{d,R}g_{Rq}^{-1} = -J_q G_d \tag{17}$$

or

$$G_{d,R}\left(\tau,\tau'\right) = -J_q\int G_d\left(\tau,\tau_1\right)g_{Rq}\left(\tau_1,\tau'\right)d\tau_1 \tag{18}$$

the minus before J_q originates from the minus in H_{sd}. The rules of analytic continuation gives

$$G_{d,R}^{<}\left(t,t'\right) = -J_q\int_{-\infty}^{\infty}dt_1[G_d^{r}\left(t,t_1\right)g_{Rq}^{<}\left(t_1,t'\right) + G_d^{<}\left(t,t_1\right)g_{Rq}^{a}\left(t_1,t'\right)] \tag{19}$$

and

$$G_{R,d}^{<}\left(t,t'\right) = -J_q\int_{-\infty}^{\infty}dt_1[g_{Rq}^{r}\left(t,t_1\right)G_d^{<}\left(t_1,t'\right) + g_{Rq}^{<}\left(t,t_1\right)G_d^{a}\left(t_1,t'\right)] \tag{20}$$

The spin current flows out of right lead is

$$\begin{aligned}
I_s &= i\sum_q J_q\left(\left\langle s_q^{+}a_q^{\dagger}\right\rangle - \left\langle a_q s_q^{-}\right\rangle\right)\\
&= -\sum_q J_q(G_{d,R}^{<}(t,t) - G_{R,d}^{<}(t,t))\\
&= 2\mathrm{Re}\sum_{\mathrm{q}}\int \mathrm{dt_1}\ \mathrm{Tr}\left[\mathrm{G_d^r}\left(\mathrm{t},\mathrm{t_1}\right)\Sigma_{\mathrm{Rq}}^{<}\left(\mathrm{t_1},\mathrm{t'}\right) + \mathrm{G_d^{<}}\left(\mathrm{t},\mathrm{t_1}\right)\Sigma_{\mathrm{Rq}}^{\mathrm{a}}\left(\mathrm{t_1},\mathrm{t'}\right)\right]
\end{aligned} \tag{21}$$

$$\Sigma_{Rq}^{\gamma}(\tau,\tau') = J_q^2 g_{Rq}^{\gamma}(\tau,\tau') \tag{22}$$

C. Calculation of G_d

Definition:

$$\begin{aligned}
G_d\left(\tau,\tau'\right) &= -i\left\langle T_c S s_q^{+}(\tau) s_q^{-}\left(\tau'\right)\right\rangle\\
&= -i\sum_{mnm'n'}\langle T_c S d_{n\uparrow}^{\dagger}d_{m\downarrow}d_{m'\downarrow}^{\dagger}d_{n'\uparrow}\rangle\delta\left(\epsilon_{n\uparrow}-\epsilon_{m\downarrow}-\omega_q\right)\delta\left(\epsilon_{n'\uparrow}-\epsilon_{m'\downarrow}-\omega_q\right)
\end{aligned} \tag{23}$$

When right lead is absent, the system Hamiltonian is

$$H = H_L + H_d + H_T. \tag{24}$$

$$G_d\left(\tau,\tau'\right) = -i\sum_{mnm'n'}G_{L,n'n\uparrow}(\tau',\tau)G_{L,mm'\downarrow}(\tau,\tau')\delta\left(\epsilon_{n\uparrow}-\epsilon_{m\downarrow}-\omega_q\right)\delta\left(\epsilon_{n'\uparrow}-\epsilon_{m'\downarrow}-\omega_q\right) \tag{25}$$

where

$$\begin{aligned}G_{L,mn\sigma}(\tau,\tau') &= -i\langle T_c d_{m\sigma}(\tau) d^\dagger_{n\sigma}(\tau')\rangle \\ &= g_{mn\sigma}(\tau,\tau')\delta_{mn} \\ &\quad + \iint d\tau_1 d\tau_2 g_{mm\sigma}(\tau,\tau_2)\sum_k t_{k\sigma n} t^*_{k\sigma m} g_{k\sigma}(\tau_2,\tau_1) g_{nn\sigma}(\tau_1,\tau') \\ &\quad + \cdots \\ &= g_{mn\sigma}(\tau,\tau')\delta_{mn} + \iint d\tau_1 d\tau_2 g_{mm\sigma}(\tau,\tau_2)\Sigma_{L,mn\sigma}(\tau_2,\tau_1) g_{nn\sigma}(\tau_1,\tau') \\ &\quad + \cdots \\ &= 1/\left[g^{-1}_{mn\sigma} - \Sigma_{L,mn\sigma}\right]\end{aligned} \tag{26}$$

$$g_{mn\sigma}(\tau,\tau') = -i\langle T_c d_{m\sigma}(\tau) d^\dagger_{n\sigma}(\tau')\rangle_0 \tag{27}$$

Self-energy of left lead

$$\Sigma_{L,mn\sigma}(\tau_2,\tau_1) = \sum_k t_{k\sigma n} t^*_{k\sigma m} g_{k\sigma}(\tau_2,\tau_1) \tag{28}$$

where

$$g_{k\sigma}(\tau_2,\tau_1) = -i\langle T_c c_{k\sigma}(\tau_2) c^\dagger_{k\sigma}(\tau_1)\rangle_0. \tag{29}$$

When left lead is absent, system Hamiltonian is

$$H = H_d + H_R + H_{sd}. \tag{30}$$

$$\begin{aligned}G_d(\tau,\tau') =& -i\sum_{mn} g_{n\uparrow}(\tau',\tau)\, g_{m\downarrow}(\tau,\tau')\,\delta(\varepsilon_{n\uparrow} - \varepsilon_{m\downarrow} - \omega_q) \\ & - \int d\tau_1 \int d\tau_2 \sum_{mnm'n'} g_{n\uparrow}(\tau_1,\tau)\, g_{m\downarrow}(\tau,\tau_1)\,\Sigma_{R,mnm'n'}(\tau_1,\tau_2)\, g_{n'\uparrow}(\tau',\tau_2)\, g_{m'\downarrow}(\tau_2,\tau') \\ & \times \delta(\varepsilon_{n\uparrow} - \varepsilon_{m\downarrow} - \omega_{q_1})\delta(\varepsilon_{n'\uparrow} - \varepsilon_{m'\downarrow} - \omega_{q_1}) \\ & + \cdots \\ =& g_d(\tau,\tau') + \iint d\tau_1 d\tau_2 g_d(\tau,\tau_1)\Sigma_R(\tau_1,\tau_2) G_d(\tau_2,\tau')\end{aligned} \tag{31}$$

in which,

$$g_d(\tau,\tau') = -i\sum_{mn} g_{n\uparrow}(\tau',\tau)\, g_{m\downarrow}(\tau,\tau')\,\delta(\varepsilon_{n\uparrow} - \varepsilon_{m\downarrow} - \omega_q), \tag{32}$$

the self-energy of right lead is

$$\Sigma_{R,mnm'n'}(\tau_1,\tau_2) = \sum_{q1} J^2_{q_1} g_{Rq_1}(\tau_1,\tau_2)\delta(\varepsilon_{n\uparrow} - \varepsilon_{m\downarrow} - \omega_{q_1})\delta(\varepsilon_{n'\uparrow} - \varepsilon_{m'\downarrow} - \omega_{q_1}) \tag{33}$$

$$g_{Rq_1}(\tau_1,\tau_2) = -i\langle T_c a_{q_1}(\tau_1) a^\dagger_{q_1}(\tau_2)\rangle_0 \tag{34}$$

Hence, when both leads are present, we have

$$\begin{aligned}G_d(\tau,\tau') =& -i\sum_{mnm'n'} G_{L,nn'\uparrow}(\tau',\tau)\, G_{L,mm'\downarrow}(\tau,\tau')\,\delta(\epsilon_{n\uparrow} - \epsilon_{m\downarrow} - \omega_q)\,\delta(\epsilon_{n'\uparrow} - \epsilon_{m'\downarrow} - \omega_q) \\ & - i\sum_{mnm'n'} G_{L,nn'\uparrow}(\tau_1,\tau)\, G_{L,mm'\downarrow}(\tau,\tau_1)\,\Sigma_{R,mnm'n'}(\tau_1,\tau_2)\, G_d(\tau_2,\tau')\,\delta(\epsilon_{n\uparrow} - \epsilon_{m\downarrow} - \omega_q) \\ & \times \delta(\epsilon_{n'\uparrow} - \epsilon_{m'\downarrow} - \omega_q)\end{aligned} \tag{35}$$

For the sack of convenience, we rewrite the above formula in matrix presentation as follows(the matrix indices are QD level indices m, n, not corrected yet!), and omit energy conservation constrain.

$$? \quad G_d(\tau,\tau') = -iG_{L\uparrow}(\tau',\tau)\, G_{L\downarrow}(\tau,\tau') - iG_{L\uparrow}(\tau_1,\tau)\, G_{L\downarrow}(\tau,\tau_1)\,\Sigma_R(\tau_1,\tau_2)\, G_d(\tau_2,\tau') \tag{36}$$

D. continuation on Eq.(35)

$$A(\tau_1,\tau') \equiv \int d\tau_2 \Sigma_R\left(\tau_1,\tau_2\right) G_d\left(\tau_2,\tau'\right) \tag{37}$$
$$B(\tau,\tau_1) \equiv G_{L\uparrow}\left(\tau_1,\tau\right) G_{L\downarrow}\left(\tau,\tau_1\right) \tag{38}$$
$$C(\tau,\tau') \equiv -iG_{L\uparrow}\left(\tau_1,\tau\right) G_{L\downarrow}\left(\tau,\tau_1\right) A(\tau_1,\tau') \rightarrow \tag{39}$$
$$C(\tau,\tau') = -i\int d\tau_1 B(\tau,\tau_1)A(\tau_1,\tau') \tag{40}$$
$$D(\tau,\tau') \equiv -iG_{L\uparrow}\left(\tau',\tau\right) G_{L\downarrow}\left(\tau,\tau'\right) \tag{41}$$

So, we have

$$G_d(\tau,\tau') = D + C \tag{42}$$

Using the analytic continuation theorem, we have

$$D^< = -iG^>_{L\uparrow}G^<_{L\downarrow} \tag{43}$$

$$C^< = -i(B^r A^< + B^< A^a) \tag{44}$$

where

$$B^r = G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow} \tag{45}$$

$$A^< = \Sigma^r_R G^<_d + \Sigma^<_R G^a_d \tag{46}$$

$$B^< = G^>_{L\uparrow}G^<_{L\downarrow} \tag{47}$$

$$A^a = \Sigma^a_R G^a_d \tag{48}$$

Then, the analytic continuation theorem on Eq.(35) yields

$$G^<_d = -iG^>_{L\uparrow}G^<_{L\downarrow} - i\left[(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow})(\Sigma^r_R G^<_d + \Sigma^<_R G^a_d) + (G^>_{L\uparrow}G^<_{L\downarrow})(\Sigma^a_R G^a_d)\right] \tag{49}$$

Similarly,

$$\begin{aligned} C^r &= -iB^r A^r \\ &= -i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow})(\Sigma^r_R G^r_d) \end{aligned} \tag{50}$$

$$D^r = -i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow}), \tag{51}$$

we have

$$\begin{aligned} G^r_d &= -i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow}) - i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow})(\Sigma^r_R G^r_d) \\ &= \frac{-i\left(G_{L\uparrow}G_{L\downarrow}\right)^r}{1 + i\left(G_{L\uparrow}G_{L\downarrow}\right)^r \Sigma^r_R} \end{aligned} \tag{52}$$

$$(G_{L\uparrow}G_{L\downarrow})^r \equiv G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow} \tag{53}$$

Now we calculate G^a_d.

$$C^a = -iB^a A^a \tag{54}$$

$$B^a = G^r_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^a_{L\downarrow} + G^r_{L\uparrow}G^a_{L\downarrow} \tag{55}$$

$$D^a = -i(G^r_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^a_{L\downarrow} + G^r_{L\uparrow}G^a_{L\downarrow}) \tag{56}$$

So we have

$$G^a_d = -i(G^r_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^a_{L\downarrow} + G^r_{L\uparrow}G^a_{L\downarrow}) - i(G^r_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^a_{L\downarrow} + G^r_{L\uparrow}G^a_{L\downarrow})(\Sigma^a_R G^a_d) \tag{57}$$

From Eq.(49) we have

$$\begin{aligned} G^<_d &= -iG^>_{L\uparrow}G^<_{L\downarrow}\left(1+\Sigma^a_R G^a_d\right) - i\left(G_{L\uparrow}G_{L\downarrow}\right)^r\left(\Sigma^<_q G^a_d + \Sigma^r_R G^<_d\right) \\ &= \frac{-iG^>_{L\uparrow}G^<_{L\downarrow}\left(1+\Sigma^a_R G^a_d\right) - i\left(G_{L\uparrow}G_{L\downarrow}\right)^r \Sigma^<_R G^a_d}{1+i\left(G_{L\uparrow}G_{L\downarrow}\right)^r\Sigma^r_R} \\ &= \frac{-iG^>_{L\uparrow}G^<_{L\downarrow}\left(1+\Sigma^a_R G^a_d\right)}{1+i\left(G_{L\uparrow}G_{L\downarrow}\right)^r\Sigma^r_R} + G^r_d\Sigma^<_R G^a_d \\ &= -i(G^r_d\Sigma^r_R+1)G^>_{L\uparrow}G^<_{L\downarrow}\left(1+\Sigma^a_R G^a_d\right) + G^r_d\Sigma^<_R G^a_d \end{aligned} \tag{58}$$

Similarly,

$$G^>_d = -i\left(G^r_d\Sigma^r_R+1\right)G^<_{L\uparrow}G^>_{L\downarrow}\left(1+\Sigma^a_R G^a_d\right) + G^r_d\Sigma^>_R G^a_d \tag{59}$$

E. DC spin current

$$I_s = 2\mathrm{Re}\sum_{\mathrm{q}}\int\frac{\mathrm{dE}}{2\pi}\,\mathrm{Tr}\left[\left(\mathrm{G}^>_{\mathrm{d}} - \mathrm{G}^<_{\mathrm{d}}\right)\Sigma^<_{\mathrm{Rq}} + \mathrm{G}^<_{\mathrm{d}}\left(\Sigma^{\mathrm{a}}_{\mathrm{Rq}} - \Sigma^{\mathrm{r}}_{\mathrm{Rq}}\right)\right] \tag{60}$$

We have

$$G^>_d(E) - G^<_d(E) = -i\left(G^r_d\Sigma^r_R+1\right)\left(G^<_{L\uparrow}G^>_{L\downarrow} - G^>_{L\uparrow}G^<_{L\downarrow}\right)\left(1+\Sigma^a_R G^a_d\right) + G^r_d\left(\Sigma^>_R - \Sigma^<_R\right)G^a_d \tag{61}$$

Fourier transformation

$$G^<_d(E) = \int_{-\infty}^{+\infty} dt G^<_d(t-t')e^{iE(t-t')} \tag{62}$$

and inverse Fourier transformation

$$G^<_d(t-t') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega G^<_d(E)e^{-iE(t-t')}, \tag{63}$$

are used, since the Green's functions only dependent on time difference. Then using Keldysh equation, we have

$$G^<_{L,mn\sigma}(E) = G^r_{L,mn\sigma}\Sigma^<_{L,mn\sigma}(E)G^a_{L,mn\sigma}(E), \tag{64}$$

where $G_{L,mn\sigma}$ is the Green's function when left free lead, QD and left coupling present. $\Sigma^<_{L,mn\sigma}$ is self-energy of left lead, defined in Eq. (29)

$$\Sigma^<_{L,mn\sigma} = if_{L\sigma}(E)\Gamma_{L,mn\sigma}(E). \tag{65}$$

so,

$$G^<_{L,mn\sigma}(E) = iG^r_{L,mn\sigma}f_{L\sigma}(E)\Gamma_{L,mn\sigma}(E)G^a_{L,mn\sigma}(E) \equiv iD_{L\sigma}f_{L\sigma}, \tag{66}$$

and

$$\begin{aligned} G^>_{L,mn\sigma}(E) &= -(G^<_{L,mn\sigma}(E))^\dagger \\ &= G^r_{L,mn\sigma}(E)\Sigma^>_{L,mn\sigma}(E)G^a_{L,mn\sigma}(E) \\ &= iD_{L\sigma}(f_{L\uparrow}(E)-1) \end{aligned} \tag{67}$$

in which, $D_{L\sigma} = G^r_{L\sigma}\Gamma_{L\sigma}G^a_{L\sigma}$, thus

$$\begin{aligned} G^<_{L\sigma}G^>_{L\sigma} - G^>_{L\sigma}G^<_{L\sigma} &= D_{L\uparrow}D_{L\downarrow}[(f_{L\uparrow}-1)f_{L\downarrow} - (f_{L\downarrow}-1)f_{L\uparrow}] \\ &= D_{L\uparrow}D_{L\downarrow}(f_{L\uparrow} - f_{L\downarrow}) \end{aligned} \tag{68}$$

$$\begin{aligned} \Sigma^<_R(E) &= \sum_{q_1} J^2_{q_1} g^<_{Rq_1}(E) \\ &= i f^B_R(E)\Gamma_R(E) \end{aligned} \tag{69}$$

$$\Sigma^a_R - \Sigma^r_R = \Sigma^<_R - \Sigma^>_R = i\Gamma_R(E). \tag{70}$$

$$G^>_d - G^<_d = -i\left[f_{L\uparrow} - f_{L\downarrow}\right]\left(G^r_d\Sigma^r_{Rq} + 1\right)D_{L\uparrow}D_{L\downarrow}\left(1 + \Sigma^a_{Rq}G^a_d\right) - iG^r_d\Gamma_{Rq}G^a_d \tag{71}$$

$$\begin{aligned} \left(G^>_d - G^<_d\right)\Sigma^<_{Rq} + G^<_d\left(\Sigma^a_{Rq} - \Sigma^r_{Rq}\right) &= \left[\left(f_{L\uparrow} - f_{L\downarrow}\right)f_R + \left(f_{L\uparrow} - 1\right)f_{L\downarrow}\right] \\ &\times \left(G^r_d\Sigma^r_{Rq} + 1\right)D_{L\uparrow}D_{L\downarrow}\left(1 + \Sigma^a_{Rq}G^a_d\right)\Gamma_{Rq} \end{aligned} \tag{72}$$

The following formula exists

$$[f_{L\uparrow}(\varepsilon) - 1]f_{L\downarrow}(\varepsilon) = -[f_{L\uparrow}(\varepsilon) - f_{L\downarrow}(\varepsilon)]f^B_L \tag{73}$$

where,

$$f_{L\sigma}(\epsilon) = \frac{1}{e^{\beta_L(\epsilon-\mu_\sigma)} + 1} \tag{74}$$

$$f^B_L = \frac{1}{e^{\beta_L\Delta\mu_s} - 1} \tag{75}$$

$\Delta\mu_s = \mu_\uparrow - \mu_\downarrow$. Note that this similar relation also exists,

$$\left(f_{L\uparrow}(\varepsilon) - 1\right)f_{L\downarrow}(\varepsilon+\omega) = -[f_{L\uparrow}(\varepsilon) - f_{L\downarrow}(\varepsilon+\omega)]f^B_L(\omega) \tag{76}$$

$$f^B_L(\varepsilon) = \frac{1}{e^{\beta_L(\omega+\Delta\mu_s)} - 1}, \tag{77}$$

is the effective Boson-Einstein distribution of left electronic lead. Eq. (72) becomes

$$\begin{aligned} \left(G^>_d - G^<_d\right)\Sigma^<_{Rq} + G^<_d\left(\Sigma^a_{Rq} - \Sigma^r_{Rq}\right) &= \left[\left(f_{L\uparrow} - f_{L\downarrow}\right)\left(f_R - f^B_L\right)\right] \\ &\times \left(G^r_d\Sigma^r_{Rq} + 1\right)D_{L\uparrow}D_{L\downarrow}\left(1 + \Sigma^a_{Rq}G^a_d\right)\Gamma_{Rq} \end{aligned} \tag{78}$$

If we assume a Ohmic spectra, $s = 1$ for

$$J_R(\omega) = \pi\alpha\omega^s\omega_c^{1-s}e^{-\omega/\omega_c} \tag{79}$$

and

$$\Sigma^r_R = -iJ_R(\omega)/2 \tag{80}$$

then

$$\Gamma_{Rq} = i(\Sigma^r_R - \Sigma^a_R) = J_R(\omega) \tag{81}$$

Substitute in Eq. (60), we get

$$I_{sR} = -\int d\omega\rho_R(\omega)\left(f_R(\omega) - f^B_L(\omega)\right)\int dE\left(f_{L\uparrow}(E) - f_{L\downarrow}(E+\omega)\right)\mathrm{Tr}[A(E,\omega)], \tag{82}$$

$$A(E,\omega) = \left[G_d^r(E)\Sigma_{Rq}^r(\omega)+1\right] D_{L\uparrow}(E)D_{L\downarrow}(E+\omega)\left[1+\Sigma_{Rq}^a(\omega)G_d^a(E)\right]\Gamma'. \tag{83}$$

Above $\rho_R(\omega)$ comes from the magnon q summation, is density of states of magnon lead, determined by magnon dispersion ω_q. Note after taking ρ out of $\Gamma_R(\omega)$, a block matrix Γ' is left in $A(E,\omega)$.

$$\Gamma' = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I_{n_{\rm wid}\times n_{\rm wid}} \end{bmatrix}, \tag{84}$$

where $I_{n_{\rm wid}\times n_{\rm wid}}$ is the unitary matrix of size $n_{\rm wid}\times n_{\rm wid}$. We have

$$\Gamma' = \Gamma'\Gamma', \tag{85}$$

so

$$\mathrm{Tr[A]} \simeq \mathrm{Tr}[\mathrm{D}\bar{\mathrm{D}}\Gamma'] \simeq \mathrm{Tr}[\Gamma'\mathrm{D}\bar{\mathrm{D}}\Gamma']. \tag{86}$$

F. Spin current from the left lead

Define spin density operator

$$N_{sk} = d_{k\uparrow}^\dagger d_{k\uparrow} - d_{k\downarrow}^\dagger d_{k\downarrow} \tag{87}$$

$$I_{sL} = (1/2)\partial_t N_s = (1/2)\left(I_\uparrow - I_\downarrow\right) \tag{88}$$

$$I_\sigma = \mathrm{Tr}\left[\left(G_{d\sigma}^r - G_{d\sigma}^a\right)\Sigma_{L\sigma}^< + G_{d\sigma}^<\left(\Sigma_{L\sigma}^a - \Sigma_{L\sigma}^r\right)\right] \tag{89}$$

$$\left[G_{d\sigma}\right]_{nm} = -i\left\langle T_c S d_{n\sigma} d_{m\sigma}^\dagger\right\rangle \tag{90}$$

the factor of 1/2 comes from spin of electron while spin of magnon is 1. Considering the continious condition of current, we should have relation $I_L + I_R = 0$.

I. LINEAR RESPONSE REGIME

$$\begin{aligned} f_R(\omega) - f_L^B(\omega) &= \frac{1}{e^{\beta_R\omega}-1} - \frac{1}{e^{\beta_L(\omega+\Delta\mu_s)}-1} \\ &= \frac{e^{\beta_L(\omega+\Delta\mu_s)} - e^{\beta_R\omega}}{[e^{\beta_R\omega}-1][e^{\beta_L(\omega+\Delta\mu_s)}-1]} \\ &= \frac{e^{\beta_L\omega}[e^{\beta_L\Delta\mu_s} - e^{(\beta_R-\beta_L)\omega}]}{e^{\beta_L\omega}[e^{(\beta_R-\beta_L)\omega} - e^{-\beta_L\omega}][e^{\beta_L(\omega+\Delta\mu_s)}-1]} \\ &= \frac{e^{\beta_L\Delta\mu_s} - e^{(\beta_R-\beta_L)\omega}}{[e^{(\beta_R-\beta_L)\omega} - e^{-\beta_L\omega}][e^{\beta_L(\omega+\Delta\mu_s)}-1]}. \end{aligned} \tag{91}$$

$$f_{L\uparrow}(E) - f_{L\downarrow}(E+\omega) = \frac{1}{e^{\beta_L(E-\mu_{L\uparrow})}+1} - \frac{1}{e^{\beta_L(E+\omega-\mu_{L\downarrow})}+1}. \tag{92}$$

Here $\Delta\mu_s = \mu_{L\uparrow} - \mu_{L\downarrow}$ as before, and $\beta_R - \beta_L = \frac{\Delta T}{k_B T_L T_R}$.

A. $\Delta\mu_s = 0$ and $\Delta T \to 0$ limit

If $\Delta\mu_s = 0$, we have

$$\begin{aligned} f_R(\omega) - f_L^B(\omega) &= \frac{e^{\beta_L \Delta\mu_s} - e^{(\beta_R-\beta_L)\omega}}{[e^{(\beta_R-\beta_L)\omega} - e^{-\beta_L\omega}][e^{\beta_L(\omega+\Delta\mu_s)} - 1]} \\ &\overset{\Delta\mu_s=0}{\longrightarrow} \frac{1 - e^{(\beta_R-\beta_L)\omega}}{[e^{(\beta_R-\beta_L)\omega} - e^{-\beta_L\omega}][e^{\beta_L\omega} - 1]} \end{aligned} \tag{93}$$

$$f_{L\uparrow}(E) - f_{L\downarrow}(E+\omega) = \frac{1}{e^{\beta_L(E-\mu_L)} + 1} - \frac{1}{e^{\beta_L(E+\omega-\mu_L)} + 1}. \tag{94}$$

In $\Delta T \to 0$ limit, $\beta_R - \beta_L \to 0$,

$$e^{(\beta_R-\beta_L)\omega} = 1 + \omega\beta_L^2 k_B \Delta T + O(\Delta T^2), \tag{95}$$

then,

$$\begin{aligned} f_R(\omega) - f_L^B(\omega) &\overset{\Delta T\to 0}{\longrightarrow} \frac{\omega k_B \beta_L^2}{[1 - e^{-\beta_L\omega}][1 - e^{\beta_L\omega}]}\Delta T \\ &\overset{\Delta T\to 0}{\longrightarrow} \frac{-\omega k_B \beta_L^2}{4\mathrm{sinh}^2(\beta_\mathrm{L}\omega/2)}\Delta T = \frac{-\omega k_B \beta_L^2}{2[\cosh(\beta_\mathrm{L}\omega) - 1]}\Delta T. \end{aligned} \tag{96}$$

Note that

$$\sinh^2(\frac{\mathrm{x}}{2}) = \frac{1}{2}[\cosh(\mathrm{x}) - 1].$$

$$f_{L\uparrow}(E) - f_{L\downarrow}(E+\omega) \overset{\Delta T\to 0}{\longrightarrow} 0. \tag{97}$$

When $\omega = 0$, the Eq. (97) is 0, thus the total coefficient is not singular.

B. $\Delta T = 0$ limit, and $\Delta\mu_s \to 0$

When $\Delta T = 0$, $\beta_R - \beta_L = 0$. The Eq. (91) reduces to

$$\begin{aligned} f_R(\omega) - f_L^B(\omega) &= \frac{e^{\beta_L \Delta\mu_s} - e^{(\beta_R-\beta_L)\omega}}{[e^{(\beta_R-\beta_L)\omega} - e^{-\beta_L\omega}][e^{\beta_L(\omega+\Delta\mu_s)} - 1]} \\ &\overset{\Delta T=0}{\longrightarrow} \frac{e^{\beta_L \Delta\mu_s} - 1}{[1 - e^{-\beta_L\omega}][e^{\beta_L(\omega+\Delta\mu_s)} - 1]} \\ &\overset{\Delta\mu_s\to 0}{\longrightarrow} \frac{e^{\beta_L \Delta\mu_s} - 1}{[1 - e^{-\beta_L\omega}][e^{\beta_L\omega} - 1]} \\ &\overset{\Delta\mu_s\to 0}{\longrightarrow} \frac{-\beta_L \Delta\mu_s}{[1 - e^{-\beta_L\omega}][1 - e^{\beta_L\omega}]} \\ &\overset{\Delta\mu_s\to 0}{\longrightarrow} \frac{\beta_L}{4\mathrm{sinh}^2(\beta_\mathrm{L}\omega/2)}\Delta\mu_s = \frac{\beta_L}{2[\cosh(\beta_\mathrm{L}\omega) - 1]}\Delta\mu_s. \end{aligned} \tag{98}$$

$$\begin{aligned} f_{L\uparrow}(E) - f_{L\downarrow}(E+\omega) &= \frac{1}{e^{\beta_L(E-\mu_{L\uparrow})} + 1} - \frac{1}{e^{\beta_L(E+\omega-\mu_{L\downarrow})} + 1} \\ &= \frac{e^{\beta_L(E+\omega-\mu_{L\downarrow})} - e^{\beta_L(E-\mu_{L\uparrow})}}{[e^{\beta_L(E-\mu_{L\uparrow})} + 1][e^{\beta_L(E+\omega-\mu_{L\downarrow})} + 1]} \\ &= \frac{\cancel{e^{\beta_L(E-\mu_{L\uparrow})}}[e^{\beta_L(\omega+\Delta\mu_s)} - 1]}{[e^{\beta_L(E-\mu_{L\uparrow})} + 1]\cancel{e^{\beta_L(E-\mu_{L\uparrow})}}[e^{\beta_L(\omega+\Delta\mu_s)} + e^{-\beta_L(E-\mu_{L\uparrow})}]} \end{aligned} \tag{99}$$

C. linear response regime

$$f_R(\omega) - f_L^B(\omega) = \frac{-\omega k_B \beta^2 \Delta T + \beta \Delta\mu_s}{2[\cosh(\beta_{\rm L}\omega) - 1]} \tag{100}$$

When $\omega \to 0$,

$$\lim_{\omega\to 0} \omega[f_R(\omega) - f_L^B(\omega)] = \frac{1}{\beta_R} - 0.$$

There is no singularity in the spin current integration if the ω in Γ_R is combined with Boson distribution.

II. TIGHT-BINDING METHOD

Tight-binding coupling t is

$$t = \frac{\hbar^2}{2ma^2},$$

in which m is the effective mass of election in the lattice, assuming $m = 0.08m_e$, which is mass of electron. a is lattice distance. $\hbar = 1.0545e - 34J \cdot s, m_e = 9.10938370e - 31\text{kg}$, so t is in unit of J.

Boltzman constant $k_B = 1.3806504^{-23} J/K, e = 1.602176634^{-19} C, \hbar = 1.0545e - 34J \cdot s, m_e = 9.10938370e - 31\text{kg}$

III. TRANSPORTATION IN A ELECTRON WAVE GUIDE

An electron wave guide is a device analogous to light wave guide, in which only small number of electron wave modes can propagate. Reference to exercise 1.3 and 1.4 in S. Datta's book. For case one, in y direction, the wave guide is constrained in a hard-well potential. $U(y < -W/2) = U(y > W/2) = \infty, U(-W/2 < y < W/2) = 0$, leads to the quantization of electron states.

$$k_y = \frac{i\pi}{W}, \qquad \text{for i is integers.} \tag{101}$$

W is the width of wave guide and central area, a is lattice constant of central lattice, $n_{\rm wid}$ is number of lattice points in y direction.

$$W = n_{\rm wid} \times a \tag{102}$$

To get a propagate wave instead of a decaying wave, the k_x must be a real number, or $k_x^2 > 0$. The total injection energy of an election is

$$E = \frac{\hbar^2(k_x^2 + k_y^2)}{2m} = \frac{\hbar^2 k_x^2}{2m} + \frac{i^2\hbar^2\pi^2}{2mW^2}. \tag{103}$$

So the threshold for ith subband or transverse mode is

$$E_i = \frac{i^2\hbar^2\pi^2}{2mW^2}, \tag{104}$$

which is 0.537 meV for first subband, effective mass $m = 0.07m_e$, and width $W = 100nm$.

IV. WAYS TO REDUCE TIME-CONSUMING

A. Low temperature

In transport problem, the Landauer type formula has term of the difference of two Fermionic distribution. Generally, this constrains the range of integrating variable to $[-\frac{T}{2}, \frac{T}{2}]$ or $[\mu_1, \mu_2]$.

B. Physical consideration

Usually, only several subbands or transverse modes are investigated, which suggests the integrating range of $[-\frac{T}{2}, E_{i+1}]$ to include i subbands, with E_i the ith subband energy threshold. When integrating a very high energy,

C. Repalcing repeating calculations by interpolation

If a complex manipulation, like matrix inverse, is contained in a loop, we can take the matrix inverse out of loop, and replace it with an interpolation of inversed matrice calculated earlier. Interpolating by

$$f(c) = \frac{f(a) - f(b)}{a - b} \times (c - a) + f(a). \tag{105}$$

D. $Tr[\Gamma'_{Rq} D_{L\uparrow}(E) D_{L\downarrow}(E+\omega)\Gamma'_{Rq}]$

Γ'_{Rq} is block matrix of dimension $n_{wid}n_{len} \times n_{wid}n_{len}$, with only $I_{n_{wid}\times n_{wid}}$ block. For n_wid=3, n_len=5, we have

$$\Gamma'_L = \begin{bmatrix} \Gamma^L_{3\times3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{106}$$

$$\Gamma'_{Rq} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I_{3\times3} \end{bmatrix}. \tag{107}$$

$$D_{L\uparrow} = G^r_{L\uparrow}\Gamma_{L\uparrow}G^a_{L\uparrow} = \begin{bmatrix} G^r_{11}\Gamma^L_{3\times3} & 0 & 0 & 0 \\ G^r_{21}\Gamma^L_{3\times3} & 0 & 0 & 0 \\ G^r_{31}\Gamma^L_{3\times3} & 0 & 0 & 0 \\ G^r_{41}\Gamma^L_{3\times3} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} G^a_{11} & G^a_{12} & G^a_{13} & G^a_{14} \\ G^a_{21} & G^a_{22} & G^a_{23} & G^a_{24} \\ G^a_{31} & G^a_{32} & G^a_{33} & G^a_{34} \\ G^a_{41} & G^a_{42} & G^a_{43} & G^a_{44} \end{bmatrix}. \tag{108}$$

Then,

$$\Gamma'_{Rq} D_{L\uparrow} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \mathrm{x} & \mathrm{x} & \mathrm{x} & \mathrm{x} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ G^r_{41}\Gamma^L_{3\times3}G^a_{11} & G^r_{41}\Gamma^L_{3\times3}G^a_{12} & G^r_{41}\Gamma^L_{3\times3}G^a_{13} & G^r_{41}\Gamma^L_{3\times3}G^a_{14} \end{bmatrix} \tag{109}$$

and

$$D_{L\downarrow}\Gamma'_{Rq} = \begin{bmatrix} 0 & 0 & 0 & \mathrm{x} \\ 0 & 0 & 0 & \mathrm{x} \\ 0 & 0 & 0 & \mathrm{x} \\ 0 & 0 & 0 & \mathrm{x} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & G^r_{11}\Gamma^L_{3\times3}G^a_{14} \\ 0 & 0 & 0 & G^r_{21}\Gamma^L_{3\times3}G^a_{14} \\ 0 & 0 & 0 & G^r_{31}\Gamma^L_{3\times3}G^a_{14} \\ 0 & 0 & 0 & G^r_{41}\Gamma^L_{3\times3}G^a_{14} \end{bmatrix} \tag{110}$$

So

$$\Gamma'_{Rq} D_{L\uparrow} D_{L\downarrow}\Gamma'_{Rq} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & A(E,\omega) \end{bmatrix}. \tag{111}$$

$$[A(E,\omega)]_{ij} = G^r_{41}\Gamma^L_{3\times3}G^a_{1i}G^r_{j1}\Gamma^L_{3\times3}G^a_{14}, \tag{112}$$

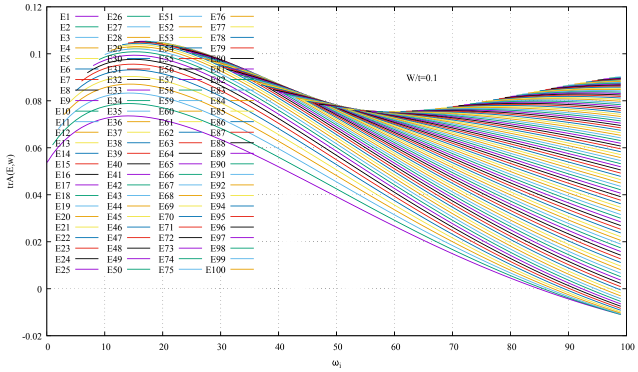

FIG. 1. TrA for the clean NM-NM-FI system.

the advanced Green's function is related to the retarded Green's function by

$$G^a = [G^r]^\dagger, \tag{113}$$

which gives

$$[A(E,\omega)]_{ij} = G^r_{41}\Gamma^L_{3\times3}[G^r]^\dagger_{1i}G^r_{j1}\Gamma^L_{3\times3}[G^r]^\dagger_{14}. \tag{114}$$

Here G^r_{ij} is a 3×3 matrix in full matrix G^r of dimension 12×12, and $\{i,j\}\in[1,2,3,4]$.

$$Tr[A(E,\omega)] = \sum_i G^r_{41}\Gamma^L_{3\times3}[G^r]^\dagger_{1i}G^r_{i1}\Gamma^L_{3\times3}[G^r]^\dagger_{14}. \tag{115}$$

E. interpolate on $Tr[A(E,\omega)]$

The interpolation to trA reduces computation from 10000 points to 1000 points.

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