# NEGF Notes

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## 0.1 Hamiltonian

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

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

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

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

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

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

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

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

### 0.1.1 check operators

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

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

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

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

## 0.2 spin current ???

$$-i\partial_{\tau'} G_{d,R}\left(\tau,\tau'\right)=\omega_q G_{d,R}\left(\tau,\tau'\right)-J_q G_d \tag{13}$$

or

$$G_{d,R}g_{Rq}^{-1}=-J_q G_d \tag{14}$$

or

$$G_{d,R}\left(\tau,\tau'\right)=-J_q\int G_d\left(\tau,\tau_1\right)g_{Rq}\left(\tau_1,\tau'\right)d\tau_1 \tag{15}$$

the minus before $J_q$ originates from the minus in $H_{sd}$. The lesser Green's function is($s_q^+$ is fermionic but $a_q$ is bosonic)

$$G_{d,R}^{<}\left(\tau,\tau'\right)=i\langle s_q^+(\tau)a_q^\dagger(\tau')\rangle \tag{16}$$

$$\begin{aligned}
I_s&=i\sum_q J_q\left(\left\langle s_q^+a_q^\dagger\right\rangle-\left\langle a_q s_q^-\right\rangle\right)\\
&=\sum_q J_q(G_{d,R}^{<}(t,t)-G_{R,d}^{<}(t,t))\\
&=-2\mathrm{Re}\sum_{\mathrm{q}}\int \mathrm{dt_1}\ \mathrm{Tr}\left[\mathrm{G_d^r}\left(\mathrm{t},\mathrm{t_1}\right)\Sigma_{\mathrm{R}}^{<}\left(\mathrm{t_1},\mathrm{t}'\right)+\mathrm{G_d^<}\left(\mathrm{t},\mathrm{t_1}\right)\Sigma_{\mathrm{R}}^{\mathrm{a}}\left(\mathrm{t_1},\mathrm{t}'\right)\right]\\
&=-2\mathrm{Re}\sum_{\mathrm{q}}\int \mathrm{dt_1}\ \mathrm{Tr}\left[\left(\mathrm{G_d^>}-\mathrm{G_d^<}\right)\Sigma_{\mathrm{Rq}}^{<}+\mathrm{G_d^<}\left(\Sigma_{\mathrm{Rq}}^{\mathrm{a}}-\Sigma_{\mathrm{Rq}}^{\mathrm{r}}\right)\right]
\end{aligned} \tag{17}$$

$$\Sigma_{Rq}(\tau,\tau')=J_q^2 g_{Rq}(\tau,\tau') \tag{18}$$

## 0.3 Calculation of $G_d$

Definition:

$$\begin{aligned}
G_d\left(\tau,\tau'\right)&=-i\left\langle T_c S s_q^+(\tau)s_q^-\left(\tau'\right)\right\rangle\\
&=-i\sum_{mnm'n'}\langle T_c S d_{n\uparrow}^\dagger d_{m\downarrow}d_{m'\downarrow}^\dagger d_{n'\uparrow}\rangle\delta\left(\epsilon_{n\uparrow}-\epsilon_{m\downarrow}-\omega_q\right)\delta\left(\epsilon_{n'\uparrow}-\epsilon_{m'\downarrow}-\omega_q\right)
\end{aligned} \tag{19}$$

When right lead is absent,

$$G_d\left(\tau,\tau'\right)=-i\sum_{mnm'n'}G_{L,n'n\uparrow}(\tau',\tau)G_{L,mm'\downarrow}(\tau,\tau')\delta\left(\epsilon_{n\uparrow}-\epsilon_{m\downarrow}-\omega_q\right)\delta\left(\epsilon_{n'\uparrow}-\epsilon_{m'\downarrow}-\omega_q\right) \tag{20}$$

where

$$\begin{aligned}
G_{L,mn\sigma}(\tau,\tau')&=-i\langle T_c d_{m\sigma}(\tau)d_{n\sigma}^\dagger(\tau')\rangle\\
&=g_{n\sigma}(\tau,\tau')\delta_{mn}\\
&\quad+\iint d\tau_1 d\tau_2 g_{m\sigma}(\tau,\tau_2)\sum_k t_{k\sigma n}t_{k\sigma m}^* g_{k\sigma}(\tau_2,\tau_1)g_{n\sigma}(\tau_1,\tau')\\
&\quad+\cdots\\
&=g_{n\sigma}(\tau,\tau')\delta_{mn}+\iint d\tau_1 d\tau_2 g_{m\sigma}(\tau,\tau_2)\Sigma_{L,mn\sigma}(\tau_2,\tau_1)g_{n\sigma}(\tau_1,\tau')\\
&\quad+\cdots\\
&=\quad ?
\end{aligned} \tag{21}$$

$$g_{n\sigma}(\tau,\tau')=-i\langle T_c d_n(\tau)d_{n\sigma}^\dagger(\tau')\rangle_0 \tag{22}$$

Self-energy of left lead

$$\Sigma_{L,mn\sigma}(\tau_2,\tau_1) = \sum_k t_{k\sigma n} t^*_{k\sigma m} g_{k\sigma}(\tau_2,\tau_1) \tag{23}$$

where

$$g_{k\sigma}(\tau_2,\tau_1) = -i\langle T_c c_{k\sigma}(\tau_2) c^\dagger_{k\sigma}(\tau_1)\rangle_0. \tag{24}$$

When left lead is absent,

$$\begin{aligned} G_d\left(\tau,\tau'\right) =& - i\sum_{mn} g_{n\uparrow}\left(\tau',\tau\right) g_{m\downarrow}\left(\tau,\tau'\right)\delta(\varepsilon_{n\uparrow}-\varepsilon_{m\downarrow}-\omega_q) \\ & - \int d\tau_1 \int d\tau_2 \sum_{mnm'n'} g_{n\uparrow}\left(\tau_1,\tau\right) g_{m\downarrow}\left(\tau,\tau_1\right) \Sigma_{R,mnm'n'}\left(\tau_1,\tau_2\right) g_{n'\uparrow}\left(\tau',\tau_2\right) g_{m'\downarrow}(\tau_2,\tau') \\ & \times \delta(\varepsilon_{n\uparrow}-\varepsilon_{m\downarrow}-\omega_{q_1})\delta(\varepsilon_{n'\uparrow}-\varepsilon_{m'\downarrow}-\omega_{q_1}) \\ & + \cdots \\ =& g_d(\tau,\tau') + \iint d\tau_1 d\tau_2 g_d(\tau,\tau_1)\Sigma_R(\tau_1,\tau_2)G_d(\tau_2,\tau') \end{aligned} \tag{25}$$

in which,

$$g_d\left(\tau,\tau'\right) = -i\sum_{mn} g_{n\uparrow}\left(\tau',\tau\right) g_{m\downarrow}\left(\tau,\tau'\right)\delta(\varepsilon_{n\uparrow}-\varepsilon_{m\downarrow}-\omega_q), \tag{26}$$

the self-energy of right lead is

$$\Sigma_{R,mnm'n'}(\tau_1,\tau_2) = -i\sum_{q1} J^2_{q_1} g_{Rq_1}(\tau_1,\tau_2)\delta(\varepsilon_{n\uparrow}-\varepsilon_{m\downarrow}-\omega_{q_1})\delta(\varepsilon_{n'\uparrow}-\varepsilon_{m'\downarrow}-\omega_{q_1}) \tag{27}$$

$$g_{Rq_1}(\tau_1,\tau_2) = -i\langle T_c a_{q_1}(\tau_1) a^\dagger_{q_1}(\tau_2)\rangle_0 \tag{28}$$

Hence, when both leads are present, we have

$$\begin{aligned} ?\ \ G_d\left(\tau,\tau'\right) =& - i\sum_{mnm'n'} G_{L,nn'\uparrow}\left(\tau',\tau\right) G_{L,mm'\downarrow}\left(\tau,\tau'\right)\delta\left(\epsilon_{n\uparrow}-\epsilon_{m\downarrow}-\omega_q\right)\delta\left(\epsilon_{n'\uparrow}-\epsilon_{m'\downarrow}-\omega_q\right) \\ & - i\sum_{mnm'n'} G_{L,nn'\uparrow}\left(\tau_1,\tau\right) G_{L,mm'\downarrow}\left(\tau,\tau_1\right)\Sigma_{R,mnm'n'}\left(\tau_1,\tau_2\right) G_d\left(\tau_2,\tau'\right)\delta\left(\epsilon_{n\uparrow}-\epsilon_{m\downarrow}-\omega_q\right) \\ & \times \delta\left(\epsilon_{n'\uparrow}-\epsilon_{m'\downarrow}-\omega_q\right) \end{aligned} \tag{29}$$

For the sack of convenience, we rewrite the above formula as follows.

$$?\ \ G_d\left(\tau,\tau'\right) = -iG_{L\uparrow}\left(\tau',\tau\right) G_{L\downarrow}\left(\tau,\tau'\right) - iG_{L\uparrow}\left(\tau_1,\tau\right) G_{L\downarrow}\left(\tau,\tau_1\right)\Sigma_R\left(\tau_1,\tau_2\right) G_d\left(\tau_2,\tau'\right) \tag{30}$$

## 0.4 continuation on Eq.(30)

$$A(\tau_1,\tau') \equiv \int d\tau_2 \Sigma_R\left(\tau_1,\tau_2\right) G_d\left(\tau_2,\tau'\right) \tag{31}$$

$$B(\tau,\tau_1) \equiv G_{L\uparrow}\left(\tau_1,\tau\right) G_{L\downarrow}\left(\tau,\tau_1\right) \tag{32}$$

$$C(\tau,\tau') \equiv -iG_{L\uparrow}\left(\tau_1,\tau\right) G_{L\downarrow}\left(\tau,\tau_1\right) A(\tau_1,\tau') \rightarrow \tag{33}$$

$$C(\tau,\tau') = -i\int d\tau_1 B(\tau,\tau_1)A(\tau_1,\tau') \tag{34}$$

$$D(\tau,\tau') \equiv -iG_{L\uparrow}\left(\tau',\tau\right) G_{L\downarrow}\left(\tau,\tau'\right) \tag{35}$$

So, we have

$$G_d(\tau, \tau') = D + C \tag{36}$$

Using the analytic continuation theorem, we have

$$D^< = -iG^>_{L\uparrow}G^<_{L\downarrow} \tag{37}$$

$$C^< = -i(B^r A^< + B^< A^a) \tag{38}$$

where

$$B^r = G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow} \tag{39}$$

$$A^< = \Sigma^r_R G^<_d + \Sigma^<_R G^a_d \tag{40}$$

$$B^< = G^>_{L\uparrow}G^<_{L\downarrow} \tag{41}$$

$$A^a = \Sigma^a_R G^a_d \tag{42}$$

Then, the analytic continuation theorem on Eq.(30) yields

$$G^<_d = -iG^>_{L\uparrow}G^<_{L\downarrow} - i\left[(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow})(\Sigma^r_R G^<_d + \Sigma^<_R G^a_d) + (G^>_{L\uparrow}G^<_{L\downarrow})(\Sigma^a_R G^a_d)\right] \tag{43}$$

Similarly,

$$\begin{aligned} C^r &= -iB^r A^r \\ &= -i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow})(\Sigma^r_R G^r_d) \end{aligned} \tag{44}$$

$$D^r = -i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow}), \tag{45}$$

we have

$$\begin{aligned} G^r_d &= -i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow}) - i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow})(\Sigma^r_R G^r_d) \\ &= \frac{-i\,(G_{L\uparrow}G_{L\downarrow})^r}{1 + i\,(G_{L\uparrow}G_{L\downarrow})^r\,\Sigma^r_R} \end{aligned} \tag{46}$$

$$(G_{L\uparrow}G_{L\downarrow})^r \equiv G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow} \tag{47}$$

Now we calculate $G^a_d$.

$$C^a = -iB^a A^a \tag{48}$$

$$B^a = G^r_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^a_{L\downarrow} + G^r_{L\uparrow}G^a_{L\downarrow} \tag{49}$$

$$D^a = -i(G^r_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^a_{L\downarrow} + G^r_{L\uparrow}G^a_{L\downarrow}) \tag{50}$$

So we have

$$G^a_d = -i(G^r_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^a_{L\downarrow} + G^r_{L\uparrow}G^a_{L\downarrow}) - i(G^r_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^a_{L\downarrow} + G^r_{L\uparrow}G^a_{L\downarrow})(\Sigma^a_R G^a_d) \tag{51}$$

From Eq.(43) we have

$$\begin{aligned} G^<_d &= -iG^>_{L\uparrow}G^<_{L\downarrow}\,(1 + \Sigma^a_R G^a_d) - i\,(G_{L\uparrow}G_{L\downarrow})^r\left(\Sigma^<_q G^a_d + \Sigma^r_R G^<_d\right) \\ &= \frac{-iG^>_{L\uparrow}G^<_{L\downarrow}\,(1 + \Sigma^a_R G^a_d) - i\,(G_{L\uparrow}G_{L\downarrow})^r\,\Sigma^<_R G^a_d}{1 + i\,(G_{L\uparrow}G_{L\downarrow})^r\,\Sigma^r_R} \\ &= \frac{-iG^>_{L\uparrow}G^<_{L\downarrow}\,(1 + \Sigma^a_R G^a_d)}{1 + i\,(G_{L\uparrow}G_{L\downarrow})^r\,\Sigma^r_R} + G^r_d\Sigma^<_R G^a_d \\ &= -i(G^r_d\Sigma^r_R + 1)G^>_{L\uparrow}G^<_{L\downarrow}\,(1 + \Sigma^a_R G^a_d) + G^r_d\Sigma^<_R G^a_d \end{aligned} \tag{52}$$

Similarly,

$$G^>_d = -i\,(G^r_d\Sigma^r_R + 1)\,G^<_{L\uparrow}G^>_{L\downarrow}\,(1 + \Sigma^a_R G^a_d) + G^r_d\Sigma^>_R G^a_d \tag{53}$$

## 0.5 DC spin current

$$
\begin{aligned}
I_s &= i\sum_q J_q\left(\left\langle s_q^+ a_q^\dagger\right\rangle - \left\langle a_q s_q^-\right\rangle\right)\\
&= \sum_q J_q(G^<_{d,R}(t,t) - G^<_{R,d}(t,t))\\
&= -2\mathrm{Re}\sum_{\mathrm{q}}\int\frac{\mathrm{dE}}{2\pi}\,\mathrm{Tr}\left[\left(\mathrm{G_d^>} - \mathrm{G_d^<}\right)\Sigma^<_{\mathrm{Rq}} + \mathrm{G_d^<}\left(\Sigma^{\mathrm{a}}_{\mathrm{Rq}} - \Sigma^{\mathrm{r}}_{\mathrm{Rq}}\right)\right]
\end{aligned}
\tag{54}
$$

We have

$$
G_d^>(E) - G_d^<(E) = -i\left(G_d^r\Sigma_R^r + 1\right)\left(G^<_{L\uparrow}G^>_{L\downarrow} - G^>_{L\uparrow}G^<_{L\downarrow}\right)\left(1 + \Sigma_R^a G_d^a\right) + G_d^r\left(\Sigma_R^> - \Sigma_R^<\right)G_d^a \tag{55}
$$

$$
\left(G_d^> - G_d^<\right)\Sigma_R^< = \left[-i\left(G_d^r\Sigma_R^r + 1\right)\left(G^<_{L\uparrow}G^>_{L\downarrow} - G^>_{L\uparrow}G^<_{L\downarrow}\right)\left(1 + \Sigma_R^a G_d^a\right) + G_d^r\left(\Sigma_R^> - \Sigma_R^<\right)G_d^a\right]\Sigma_R^< \tag{56}
$$

Fourier transformation

$$
G_d^<(E) = \int_{-\infty}^{+\infty} dt G_d^<(t-t')e^{iE(t-t')} \tag{57}
$$

and inverse Fourier transformation

$$
G_d^<(t-t') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega G_d^<(E)e^{-iE(t-t')}, \tag{58}
$$

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

$$
G^<_{L,mn\sigma}(E) = G^r_{L,mn\sigma}\Sigma^<_{L,mn\sigma}(E)G^a_{L,mn\sigma}(E), \tag{59}
$$

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. (24)

$$
\Sigma^<_{L,mn\sigma} = if_{L\sigma}(E)\Gamma_{L,mn\sigma}(E). \tag{60}
$$

so,

$$
G^<_{L,mn\sigma}(E) = iG^r_{L,mn\sigma}f_{L\sigma}(E)\Gamma_{L,mn\sigma}(E)G^a_{L,mn\sigma}(E) \equiv iD_{L\sigma}f_{L\sigma}, \tag{61}
$$

and

$$
\begin{aligned}
G^>_{L,mn\sigma}(E) &= -(G^<_{L,mn\sigma}(E))^\dagger\\
&= G^r_{L,mn\sigma}(E)\Sigma^>_{L,mn\sigma}(E)G^a_{L,mn\sigma}(E)\\
&= iD_{L\sigma}(f_{L\uparrow}(E) - 1)
\end{aligned}
\tag{62}
$$

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

$$
\begin{aligned}
\Sigma_R^<(E) &= \sum_{q_1} J^2_{q_1} g^<_{Rq_1}(E)\\
&= if_R^B(E)\Gamma_R(E)
\end{aligned}
\tag{63}
$$

$$
\Sigma_R^a - \Sigma_R^r = \Sigma_R^< - \Sigma_R^> = i\Gamma_R(E). \tag{64}
$$

$$
G_d^> - G_d^< = i\left[f_{L\uparrow} - f_{L\downarrow}\right]\left(G_d^r\Sigma^r_{Rq} + 1\right)D_{L\uparrow}D_{L\downarrow}\left(1 + \Sigma^a_{Rq}G_d^a\right) - iG_d^r\Gamma_{Rq}G_d^a \tag{65}
$$

$$
\begin{aligned}
\left(G_d^> - G_d^<\right)\Sigma^<_{Rq} + G_d^<\left(\Sigma^a_{Rq} - \Sigma^r_{Rq}\right) = &-\left[\left(f_{L\uparrow} - f_{L\downarrow}\right)f_R + \left(f_{L\uparrow} - 1\right)f_{L\downarrow}\right]\\
&\times\left(G_d^r\Sigma^r_{Rq} + 1\right)D_{L\uparrow}D_{L\downarrow}\left(1 + \Sigma^a_{Rq}G_d^a\right)\Gamma_{Rq}
\end{aligned}
\tag{66}
$$

The following formula exists

$$\left(f_{L\uparrow}-1\right)f_{L\downarrow}=-\left(f_{L\uparrow}-f_{L\downarrow}\right)f_L^B \tag{67}$$

where,

$$f_{L\sigma}(\epsilon)=\frac{1}{e^{\beta_L(\epsilon-\mu_\sigma)}+1} \tag{68}$$

$$f_L^B=\frac{1}{e^{\beta_L\Delta\mu_s}-1} \tag{69}$$

$\Delta\mu_s=\mu_\uparrow-\mu_\downarrow$ ($\omega=\varepsilon_\downarrow-\varepsilon_\uparrow$?). Substitute in Eq. (54), we get

### 0.6 Spin current from the left lead

Define spin density operator

$$N_{sk}=d_{k\uparrow}^\dagger d_{k\uparrow}-d_{k\downarrow}^\dagger d_{k\downarrow} \tag{70}$$

$$I_{sL}=(1/2)\partial_t N_s=(1/2)\left(I_\uparrow-I_\downarrow\right) \tag{71}$$

$$I_\sigma=\mathrm{Tr}\left[\left(G_{d\sigma}^r-G_{d\sigma}^a\right)\Sigma_{L\sigma}^<+G_{d\sigma}^<\left(\Sigma_{L\sigma}^a-\Sigma_{L\sigma}^r\right)\right] \tag{72}$$

$$\left[G_{d\sigma}\right]_{nm}=-i\left\langle T_c S d_{n\sigma}d_{m\sigma}^\dagger\right\rangle \tag{73}$$

the factor of 1/2 comes from spin of electron while spin of magnon is 1.

## References

[1] Y, K, Kato. Observation of the Spin Hall Effect in Semiconductors[J]. Science, 2004.

[2] Cao Zhan, Investigation on DC electronic transport in hybrid multiterminal quantum dot systems[D], 2017.