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}.

$$\begin{aligned}
I_s&=i\sum_q J_q\left(\left\langle s_q^+a_q^\dagger\right\rangle-\left\langle a_q s_q^-\right\rangle\right)\\
&=\sum_q J_q(G^<_{d,R}(t,t')-G^<_{R,d}(t,t'))\\
&=-2\mathrm{Re}\sum_{\mathrm{q}}\int\mathrm{Tr}\left[\mathrm{G_d^r}\left(\mathrm{t,t_1}\right)\Sigma_\mathrm{R}^<\left(\mathrm{t_1,t'}\right)+\mathrm{G_d^<}\left(\mathrm{t,t_1}\right)\Sigma_\mathrm{R}^\mathrm{a}\left(\mathrm{t_1,t'}\right)\right]\mathrm{dt_1}\\
&=-2\mathrm{Re}\sum_{\mathrm{q}}\int\mathrm{Tr}\left[\left(\mathrm{G_d^>}-\mathrm{G_d^<}\right)\Sigma_\mathrm{Rq}^<+\mathrm{G_d^<}\left(\Sigma_\mathrm{Rq}^\mathrm{a}-\Sigma_\mathrm{Rq}^\mathrm{r}\right)\right]\mathrm{dt_1}
\end{aligned} \tag{16}$$

$$\Sigma_{Rq}(\tau,\tau')=J_q^2 g_{Rq}(\tau,\tau') \tag{17}$$

0.3 Calculation of G_d

Definition:

$$\begin{aligned}
G_d\left(\tau,\tau'\right)&=-i\left\langle T_c S s_q^+(\tau)s_q^-\left(\tau'\right)\right\rangle\\
&=-i\sum_{mnm'n'}\langle T_c S d^\dagger_{n\uparrow}d_{m\downarrow}d^\dagger_{m'\downarrow}d_{n'\uparrow}\rangle\delta\left(\epsilon_{n\uparrow}-\epsilon_{m\downarrow}-\omega_q\right)\delta\left(\epsilon_{n'\uparrow}-\epsilon_{m'\downarrow}-\omega_q\right)
\end{aligned} \tag{18}$$

When right lead is absent,

$$G_d\left(\tau,\tau'\right)=-i\sum_{mnm'n'}G_{L,n'n\uparrow}(\tau',\tau)G_{L,mm'\downarrow}(\tau,\tau')\delta\left(\epsilon_{n\uparrow}-\epsilon_{m\downarrow}-\omega_q\right)\delta\left(\epsilon_{n'\uparrow}-\epsilon_{m'\downarrow}-\omega_q\right) \tag{19}$$

where

$$\begin{aligned}
G_{L,mn\sigma}(\tau,\tau')&=-i\langle T_c d_{m\sigma}(\tau)d^\dagger_{n\sigma}(\tau')\rangle\\
&=g_{n\sigma}(\tau,\tau')\delta_{mn}\\
&\quad+\iint d\tau_1 d\tau_2 g_{m\sigma}(\tau,\tau_2)\sum_k t_{k\sigma n}t^*_{k\sigma m}g_{k\sigma}(\tau_2,\tau_1)g_{n\sigma}(\tau_1,\tau')\\
&\quad+\cdots\\
&=g_{n\sigma}(\tau,\tau')\delta_{mn}+\iint d\tau_1 d\tau_2 g_{m\sigma}(\tau,\tau_2)\Sigma_{L,mn\sigma}(\tau_2,\tau_1)g_{n\sigma}(\tau_1,\tau')\\
&\quad+\cdots\\
&=\quad ?
\end{aligned} \tag{20}$$

$$g_{n\sigma}(\tau,\tau')=-i\langle T_c d_n(\tau)d^\dagger_{n\sigma}(\tau')\rangle_0 \tag{21}$$

Self-energy of left lead

$$\Sigma_{L,mn\sigma}(\tau_2,\tau_1)=\sum_k t_{k\sigma n}t^*_{k\sigma m}g_{k\sigma}(\tau_2,\tau_1) \tag{22}$$

where

$$g_{k\sigma}(\tau_2,\tau_1) = -i\langle T_c c_{k\sigma}(\tau_2) c^\dagger_{k\sigma}(\tau_1)\rangle_0 \tag{23}$$

When left lead is absent,

$$\begin{aligned}
G_d\left(\tau,\tau'\right) =& -i\sum_{mn} g_{n\uparrow}\left(\tau',\tau\right) g_{m\downarrow}\left(\tau,\tau'\right)\delta(\varepsilon_{n\uparrow}-\varepsilon_{m\downarrow}-\omega_q) \\
& - \int d\tau_1 \int d\tau_2 \sum_{mnm'n'} g_{n\uparrow}\left(\tau_1,\tau\right) g_{m\downarrow}\left(\tau,\tau_1\right)\Sigma_{R,mnm'n'}\left(\tau_1,\tau_2\right) g_{n'\uparrow}\left(\tau',\tau_2\right) g_{m'\downarrow}(\tau_2,\tau') \\
& \quad \times \delta(\varepsilon_{n\uparrow}-\varepsilon_{m\downarrow}-\omega_{q_1})\delta(\varepsilon_{n'\uparrow}-\varepsilon_{m'\downarrow}-\omega_{q_1}) \\
& + \cdots \\
=& g_d(\tau,\tau') + \iint d\tau_1 d\tau_2 g_d(\tau,\tau_1)\Sigma_R(\tau_1,\tau_2)G_d(\tau_2,\tau')
\end{aligned} \tag{24}$$

in which,

$$g_d\left(\tau,\tau'\right) = -i\sum_{mn} g_{n\uparrow}\left(\tau',\tau\right) g_{m\downarrow}\left(\tau,\tau'\right)\delta(\varepsilon_{n\uparrow}-\varepsilon_{m\downarrow}-\omega_q), \tag{25}$$

the self-energy of right lead is

$$\Sigma_{R,mnm'n'}(\tau_1,\tau_2) = -i\sum_{q1} J^2_{q_1} g_{Rq_1}(\tau_1,\tau_2)\delta(\varepsilon_{n\uparrow}-\varepsilon_{m\downarrow}-\omega_{q_1})\delta(\varepsilon_{n'\uparrow}-\varepsilon_{m'\downarrow}-\omega_{q_1}) \tag{26}$$

$$g_{Rq_1}(\tau_1,\tau_2) = -i\langle T_c a_{q_1}(\tau_1) a^\dagger_{q_1}(\tau_2)\rangle_0 \tag{27}$$

Hence, when both leads are present, we have

$$\begin{aligned}
? \quad G_d\left(\tau,\tau'\right) =& -i\sum_{mnm'n'} G_{L,nn'\uparrow}\left(\tau',\tau\right) G_{L,mm'\downarrow}\left(\tau,\tau'\right)\delta\left(\epsilon_{n\uparrow}-\epsilon_{m\downarrow}-\omega_q\right)\delta\left(\epsilon_{n'\uparrow}-\epsilon_{m'\downarrow}-\omega_q\right) \\
& - i\sum_{mnm'n'} G_{L,nn'\uparrow}\left(\tau_1,\tau\right) G_{L,mm'\downarrow}\left(\tau,\tau_1\right)\Sigma_{R,mnm'n'}\left(\tau_1,\tau_2\right) G_d\left(\tau_2,\tau'\right)\delta\left(\epsilon_{n\uparrow}-\epsilon_{m\downarrow}-\omega_q\right) \\
& \quad \times \delta\left(\epsilon_{n'\uparrow}-\epsilon_{m'\downarrow}-\omega_q\right)
\end{aligned} \tag{28}$$

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

$$? \quad G_d\left(\tau,\tau'\right) = -iG_{L\uparrow}\left(\tau',\tau\right) G_{L\downarrow}\left(\tau,\tau'\right) - iG_{L\uparrow}\left(\tau_1,\tau\right) G_{L\downarrow}\left(\tau,\tau_1\right)\Sigma_R\left(\tau_1,\tau_2\right) G_d\left(\tau_2,\tau'\right) \tag{29}$$

0.4 continuation on Eq.(29)

$$A(\tau_1,\tau') \equiv \int d\tau_2 \Sigma_R\left(\tau_1,\tau_2\right) G_d\left(\tau_2,\tau'\right) \tag{30}$$

$$B(\tau,\tau_1) \equiv G_{L\uparrow}\left(\tau_1,\tau\right) G_{L\downarrow}\left(\tau,\tau_1\right) \tag{31}$$

$$C(\tau,\tau') \equiv -iG_{L\uparrow}\left(\tau_1,\tau\right) G_{L\downarrow}\left(\tau,\tau_1\right) A(\tau_1,\tau') \rightarrow \tag{32}$$

$$C(\tau,\tau') = -i\int d\tau_1 B(\tau,\tau_1)A(\tau_1,\tau') \tag{33}$$

$$D(\tau,\tau') \equiv -iG_{L\uparrow}\left(\tau',\tau\right) G_{L\downarrow}\left(\tau,\tau'\right) \tag{34}$$

So, we have

$$G_d(\tau,\tau') = D + C \tag{35}$$

Using the analytic continuation theorem, we have

$$D^< = -iG^>_{L\uparrow}G^<_{L\downarrow} \tag{36}$$

$$C^< = -i(B^r A^< + B^< A^a) \tag{37}$$

where

$$B^r = G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow} \tag{38}$$

$$A^< = \Sigma^r_R G^<_d + \Sigma^<_R G^a_d \tag{39}$$

$$B^< = G^>_{L\uparrow}G^<_{L\downarrow} \tag{40}$$

$$A^a = \Sigma^a_R G^a_d \tag{41}$$

Then, the analytic continuation theorem on Eq.(29) yields

$$G^<_d = -iG^>_{L\uparrow}G^<_{L\downarrow} - i\left[(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow})(\Sigma^r_R G^<_d + \Sigma^<_R G^a_d) + (G^>_{L\uparrow}G^<_{L\downarrow})(\Sigma^a_R G^a_d)\right] \tag{42}$$

Similarly,

$$\begin{aligned} C^r &= -iB^r A^r \\ &= -i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow})(\Sigma^r_R G^r_d) \end{aligned} \tag{43}$$

$$D^r = -i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow}), \tag{44}$$

we have

$$\begin{aligned} G^r_d &= -i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow}) - i(G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow})(\Sigma^r_R G^r_d) \\ &= \frac{-i\left(G_{L\uparrow}G_{L\downarrow}\right)^r}{1 + i\left(G_{L\uparrow}G_{L\downarrow}\right)^r \Sigma^r_R} \end{aligned} \tag{45}$$

$$\left(G_{L\uparrow}G_{L\downarrow}\right)^r \equiv G^a_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^r_{L\downarrow} + G^a_{L\uparrow}G^r_{L\downarrow} \tag{46}$$

Now we calculate G^a_d.

$$C^a = -iB^a A^a \tag{47}$$

$$B^a = G^r_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^a_{L\downarrow} + G^r_{L\uparrow}G^a_{L\downarrow} \tag{48}$$

$$D^a = -i(G^r_{L\uparrow}G^<_{L\downarrow} + G^>_{L\uparrow}G^a_{L\downarrow} + G^r_{L\uparrow}G^a_{L\downarrow}) \tag{49}$$

So we have

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

From Eq.(42) we have

$$\begin{aligned} G^<_d &= -iG^>_{L\uparrow}G^<_{L\downarrow}\left(1 + \Sigma^a_R G^a_d\right) - i\left(G_{L\uparrow}G_{L\downarrow}\right)^r \left(\Sigma^<_q G^a_d + \Sigma^r_R G^<_d\right) \\ &= \frac{-iG^>_{L\uparrow}G^<_{L\downarrow}\left(1 + \Sigma^a_R G^a_d\right) - i\left(G_{L\uparrow}G_{L\downarrow}\right)^r \Sigma^<_R G^a_d}{1 + i\left(G_{L\uparrow}G_{L\downarrow}\right)^r \Sigma^r_R} \\ &= \frac{-iG^>_{L\uparrow}G^<_{L\downarrow}\left(1 + \Sigma^a_R G^a_d\right)}{1 + i\left(G_{L\uparrow}G_{L\downarrow}\right)^r \Sigma^r_R} + G^r_d \Sigma^<_R G^a_d \\ &= -i(G^r_d \Sigma^r_R + 1)G^>_{L\uparrow}G^<_{L\downarrow}\left(1 + \Sigma^a_R G^a_d\right) + G^r_d \Sigma^<_R G^a_d \end{aligned} \tag{51}$$

Similarly,

$$G^>_d = -i\left(G^r_d \Sigma^r_R + 1\right) G^<_{L\uparrow}G^>_{L\downarrow}\left(1 + \Sigma^a_R G^a_d\right) + G^r_d \Sigma^>_R G^a_d \tag{52}$$

0.5 DC spin current

We have

$$G_d^>(E) - G_d^<(E) = -i\left(G_d^r \Sigma_R^r + 1\right)\left(G_{L\uparrow}^< G_{L\downarrow}^> - G_{L\uparrow}^> G_{L\downarrow}^<\right)\left(1 + \Sigma_R^a G_d^a\right) + G_d^r\left(\Sigma_R^> - \Sigma_R^<\right) G_d^a \tag{53}$$

$$\left(G_d^> - G_d^<\right)\Sigma_R^< = \left[-i\left(G_d^r \Sigma_R^r + 1\right)\left(G_{L\uparrow}^< G_{L\downarrow}^> - G_{L\uparrow}^> G_{L\downarrow}^<\right)\left(1 + \Sigma_R^a G_d^a\right) + G_d^r\left(\Sigma_R^> - \Sigma_R^<\right) G_d^a\right]\Sigma_R^< \tag{54}$$

Fourier transformation

$$G_d^<(E) = \int_{-\infty}^{+\infty} dt G_d^<(t-t') e^{iE(t-t')} \tag{55}$$

and inverse Fourier transformation

$$G_d^<(t-t') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega G_d^<(E) e^{-iE(t-t')} \tag{56}$$

Then,

$$G_{L,mn\uparrow}(E) = \tag{57}$$

$$G_{L\uparrow}^> = 1 - f_{L\uparrow} \tag{58}$$

$$G_{L\downarrow}^< = f_{L\downarrow} \tag{59}$$

$$\Sigma_R^<(t,t') = -i\sum_{q_1} J_{q_1}^2 g_{Rq_1}^<(t,t') \tag{60}$$

$$\Sigma_R^a - \Sigma_R^r = \tag{61}$$

$$G_d^<\left(\Sigma_{Rq}^a - \Sigma_{Rq}^r\right) = \tag{62}$$

$$? \quad G_{L\sigma}^< = iG_{L\sigma}^r \Gamma_{L\sigma} f_{L\sigma} G_{L\sigma}^a \equiv iD_{L\sigma} f_{L\sigma} \tag{63}$$

The following formula exists

$$\left(f_{L\uparrow} - 1\right) f_{L\downarrow} = -\left(f_{L\uparrow} - f_{L\downarrow}\right) f_L^B \tag{64}$$

where,

$$f_{L\sigma}(\epsilon) = \frac{1}{\exp\left(\beta_L\left(\epsilon - \mu_\sigma\right)\right) + 1} \tag{65}$$

$$f_L^B(\omega) = \frac{1}{\exp\left(\beta_L\left(\omega + \Delta\mu_s\right)\right) - 1} \tag{66}$$

and $\omega = \varepsilon_\downarrow - \varepsilon_\uparrow, \Delta\mu_s = \mu_\uparrow - \mu_\downarrow$.

0.6 Spin current from the left lead

Define spin density operator

$$N_{sk} = d_{k\uparrow}^\dagger d_{k\uparrow} - d_{k\downarrow}^\dagger d_{k\downarrow} \tag{67}$$

$$I_{sL} = (1/2)\partial_t N_s = (1/2)\left(I_\uparrow - I_\downarrow\right) \tag{68}$$

$$I_\sigma = \mathrm{Tr}\left[\left(G_{d\sigma}^r - G_{d\sigma}^a\right)\Sigma_{L\sigma}^< + G_{d\sigma}^<\left(\Sigma_{L\sigma}^a - \Sigma_{L\sigma}^r\right)\right] \tag{69}$$

$$\left[G_{d\sigma}\right]_{nm} = -i\left\langle T_c S d_{n\sigma} d_{m\sigma}^\dagger\right\rangle \tag{70}$$

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.