

NEGF Notes

November 4, 2020

0.1 Hamiltonian

$$H = H_L + H_R + H_d + H_T + H_{sd} \quad (1)$$

$$H_L = \sum_{k\sigma} \epsilon_{k\sigma,L} c_{k\sigma}^\dagger c_{k\sigma} \quad (2)$$

$$H_R = \sum_q \omega_q a_q^\dagger a_q \quad (3)$$

$$H_d = \sum_{n\sigma} \epsilon_{n\sigma} d_{n\sigma}^\dagger d_{n\sigma} \quad (4)$$

$$H_T = \sum_{k\sigma n} \left(t_{k\sigma n} c_{k\sigma}^\dagger d_{n\sigma} + t_{k\sigma n}^* d_{n\sigma}^\dagger c_{k\sigma} \right) \quad (5)$$

$$H_{sd} = - \sum_{qnm} J_q \left(d_{n\uparrow}^\dagger d_{m\downarrow} a_q^\dagger + a_q d_{m\downarrow}^\dagger d_{n\uparrow} \right) \delta(\epsilon_{n\uparrow} - \epsilon_{m\downarrow} - \omega_q) \quad (6)$$

$$s_q^+ = \sum_{nm} d_{n\uparrow}^\dagger d_{m\downarrow} \delta_{\uparrow\downarrow} \quad (7)$$

$$s_q^- = \sum_{nm} d_{m\downarrow}^\dagger d_{n\uparrow} \delta_{\uparrow\downarrow} \quad (8)$$

0.1.1 check operators

$$i\dot{a}_q = \omega_q a_q - J_q s_q^+ \quad (9)$$

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

$$i\dot{d}_{n\uparrow} = \epsilon_{n\uparrow} d_{n\uparrow} + \sum_k t_{k\uparrow n}^* c_{k\uparrow} - \sum_{q,m} J_q a_q^\dagger d_{m\downarrow} \delta(\epsilon_{n\uparrow} - \epsilon_{m\downarrow} - \omega_q) \quad (11)$$

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

0.2 spin current ???

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

or

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

or

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

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)

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

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

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

0.3 Calculation of G_d

Definition:

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

When right lead is absent,

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

where

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

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

Self-energy of left lead

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

where

$$g_{k\sigma}(\tau_2, \tau_1) = -i \langle T_c c_{k\sigma}(\tau_2) c_{k\sigma}^\dagger(\tau_1) \rangle_0 \quad (24)$$

When left lead is absent,

$$\begin{aligned} G_d(\tau, \tau') &= -i \sum_{mn} g_{n\uparrow}(\tau', \tau) g_{m\downarrow}(\tau, \tau') \delta(\varepsilon_{n\uparrow} - \varepsilon_{m\downarrow} - \omega_q) \\ &\quad - \int d\tau_1 \int d\tau_2 \sum_{mnm'n'} g_{n\uparrow}(\tau_1, \tau) g_{m\downarrow}(\tau, \tau_1) \Sigma_{R,mnm'n'}(\tau_1, \tau_2) g_{n'\uparrow}(\tau', \tau_2) g_{m'\downarrow}(\tau_2, \tau') \\ &\quad \times \delta(\varepsilon_{n\uparrow} - \varepsilon_{m\downarrow} - \omega_{q1}) \delta(\varepsilon_{n'\uparrow} - \varepsilon_{m'\downarrow} - \omega_{q1}) \\ &\quad + \dots \\ &= g_d(\tau, \tau') + \iint d\tau_1 d\tau_2 g_d(\tau, \tau_1) \Sigma_R(\tau_1, \tau_2) G_d(\tau_2, \tau') \end{aligned} \quad (25)$$

in which,

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

the self-energy of right lead is

$$\Sigma_{R,mnm'n'}(\tau_1, \tau_2) = -i \sum_{q1} J_{q1}^2 g_{Rq1}(\tau_1, \tau_2) \delta(\varepsilon_{n\uparrow} - \varepsilon_{m\downarrow} - \omega_{q1}) \delta(\varepsilon_{n'\uparrow} - \varepsilon_{m'\downarrow} - \omega_{q1}) \quad (27)$$

$$g_{Rq1}(\tau_1, \tau_2) = -i \langle T_c a_{q1}(\tau_1) a_{q1}^\dagger(\tau_2) \rangle_0 \quad (28)$$

Hence, when both leads are present, we have

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

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

$$? \quad G_d(\tau, \tau') = -i G_{L\uparrow}(\tau', \tau) G_{L\downarrow}(\tau, \tau') - i G_{L\uparrow}(\tau_1, \tau) G_{L\downarrow}(\tau, \tau_1) \Sigma_R(\tau_1, \tau_2) G_d(\tau_2, \tau') \quad (30)$$

0.4 continuation on Eq.(30)

$$A(\tau_1, \tau') \equiv \int d\tau_2 \Sigma_R(\tau_1, \tau_2) G_d(\tau_2, \tau') \quad (31)$$

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

$$C(\tau, \tau') \equiv -i G_{L\uparrow}(\tau_1, \tau) G_{L\downarrow}(\tau, \tau_1) A(\tau_1, \tau') \rightarrow \quad (33)$$

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

$$D(\tau, \tau') \equiv -i G_{L\uparrow}(\tau', \tau) G_{L\downarrow}(\tau, \tau') \quad (35)$$

So, we have

$$G_d(\tau, \tau') = D + C \quad (36)$$

Using the analytic continuation theorem, we have

$$D^< = -iG_{L\uparrow}^>G_{L\downarrow}^< \quad (37)$$

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

where

$$B^r = G_{L\uparrow}^a G_{L\downarrow}^< + G_{L\uparrow}^> G_{L\downarrow}^r + G_{L\uparrow}^a G_{L\downarrow}^r \quad (39)$$

$$A^< = \Sigma_R^r G_d^< + \Sigma_R^< G_d^a \quad (40)$$

$$B^< = G_{L\uparrow}^> G_{L\downarrow}^< \quad (41)$$

$$A^a = \Sigma_R^a G_d^a \quad (42)$$

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

$$G_d^< = -iG_{L\uparrow}^>G_{L\downarrow}^< - i \left[(G_{L\uparrow}^a G_{L\downarrow}^< + G_{L\uparrow}^> G_{L\downarrow}^r + G_{L\uparrow}^a G_{L\downarrow}^r) (\Sigma_R^r G_d^< + \Sigma_R^< G_d^a) + (G_{L\uparrow}^> G_{L\downarrow}^<) (\Sigma_R^a G_d^a) \right] \quad (43)$$

Similarly,

$$\begin{aligned} C^r &= -iB^r A^r \\ &= -i(G_{L\uparrow}^a G_{L\downarrow}^< + G_{L\uparrow}^> G_{L\downarrow}^r + G_{L\uparrow}^a G_{L\downarrow}^r) (\Sigma_R^r G_d^r) \end{aligned} \quad (44)$$

$$D^r = -i(G_{L\uparrow}^a G_{L\downarrow}^< + G_{L\uparrow}^> G_{L\downarrow}^r + G_{L\uparrow}^a G_{L\downarrow}^r), \quad (45)$$

we have

$$\begin{aligned} G_d^r &= -i(G_{L\uparrow}^a G_{L\downarrow}^< + G_{L\uparrow}^> G_{L\downarrow}^r + G_{L\uparrow}^a G_{L\downarrow}^r) - i(G_{L\uparrow}^a G_{L\downarrow}^< + G_{L\uparrow}^> G_{L\downarrow}^r + G_{L\uparrow}^a G_{L\downarrow}^r) (\Sigma_R^r G_d^r) \\ &= \frac{-i(G_{L\uparrow} G_{L\downarrow})^r}{1 + i(G_{L\uparrow} G_{L\downarrow})^r \Sigma_R^r} \end{aligned} \quad (46)$$

$$(G_{L\uparrow} G_{L\downarrow})^r \equiv G_{L\uparrow}^a G_{L\downarrow}^< + G_{L\uparrow}^> G_{L\downarrow}^r + G_{L\uparrow}^a G_{L\downarrow}^r \quad (47)$$

Now we calculate G_d^a .

$$C^a = -iB^a A^a \quad (48)$$

$$B^a = G_{L\uparrow}^r G_{L\downarrow}^< + G_{L\uparrow}^> G_{L\downarrow}^a + G_{L\uparrow}^r G_{L\downarrow}^a \quad (49)$$

$$D^a = -i(G_{L\uparrow}^r G_{L\downarrow}^< + G_{L\uparrow}^> G_{L\downarrow}^a + G_{L\uparrow}^r G_{L\downarrow}^a) \quad (50)$$

So we have

$$G_d^a = -i(G_{L\uparrow}^r G_{L\downarrow}^< + G_{L\uparrow}^> G_{L\downarrow}^a + G_{L\uparrow}^r G_{L\downarrow}^a) - i(G_{L\uparrow}^r G_{L\downarrow}^< + G_{L\uparrow}^> G_{L\downarrow}^a + G_{L\uparrow}^r G_{L\downarrow}^a) (\Sigma_R^a G_d^a) \quad (51)$$

From Eq.(43) we have

$$\begin{aligned} G_d^< &= -iG_{L\uparrow}^>G_{L\downarrow}^< (1 + \Sigma_R^a G_d^a) - i(G_{L\uparrow} G_{L\downarrow})^r (\Sigma_q^< G_d^a + \Sigma_R^r G_d^<) \\ &= \frac{-iG_{L\uparrow}^>G_{L\downarrow}^< (1 + \Sigma_R^a G_d^a) - i(G_{L\uparrow} G_{L\downarrow})^r \Sigma_R^< G_d^a}{1 + i(G_{L\uparrow} G_{L\downarrow})^r \Sigma_R^r} \\ &= \frac{-iG_{L\uparrow}^>G_{L\downarrow}^< (1 + \Sigma_R^a G_d^a)}{1 + i(G_{L\uparrow} G_{L\downarrow})^r \Sigma_R^r} + G_d^r \Sigma_R^< G_d^a \\ &= -i(G_d^r \Sigma_R^r + 1) G_{L\uparrow}^> G_{L\downarrow}^< (1 + \Sigma_R^a G_d^a) + G_d^r \Sigma_R^< G_d^a \end{aligned} \quad (52)$$

Similarly,

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

0.5 DC spin current

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

We have

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

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

Fourier transformation

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

and inverse Fourier transformation

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

Then,

$$G_{L,mn\uparrow}(E) = \tag{59}$$

$$G_{L\uparrow}^> = 1 - f_{L\uparrow} \tag{60}$$

$$G_{L\downarrow}^< = f_{L\downarrow} \tag{61}$$

$$\Sigma_R^<(t, t') = -i \sum_{q1} J_{q1}^2 g_{Rq1}^<(t, t') \tag{62}$$

$$\Sigma_R^a - \Sigma_R^r = \tag{63}$$

$$G_d^< (\Sigma_{Rq}^a - \Sigma_{Rq}^r) = \tag{64}$$

$$? \quad G_{L\sigma}^< = i G_{L\sigma}^r \Gamma_{L\sigma} f_{L\sigma} G_{L\sigma}^a \equiv i D_{L\sigma} f_{L\sigma} \tag{65}$$

The following formula exists

$$(f_{L\uparrow} - 1) f_{L\downarrow} = - (f_{L\uparrow} - f_{L\downarrow}) f_L^B \tag{66}$$

where,

$$f_{L\sigma}(\epsilon) = \frac{1}{\exp(\beta_L(\epsilon - \mu_\sigma)) + 1} \tag{67}$$

$$f_L^B(\omega) = \frac{1}{\exp(\beta_L(\omega + \Delta\mu_s)) - 1} \tag{68}$$

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

$$N_{sk} = d_{k\uparrow}^\dagger d_{k\uparrow} - d_{k\downarrow}^\dagger d_{k\downarrow} \tag{69}$$

$$I_{sL} = (1/2) \partial_t N_s = (1/2) (I_\uparrow - I_\downarrow) \tag{70}$$

$$I_\sigma = \text{Tr} [(G_{d\sigma}^r - G_{d\sigma}^a) \Sigma_{L\sigma}^< + G_{d\sigma}^< (\Sigma_{L\sigma}^a - \Sigma_{L\sigma}^r)] \tag{71}$$

$$[G_{d\sigma}]_{nm} = -i \langle T_c S d_{n\sigma} d_{m\sigma}^\dagger \rangle \tag{72}$$

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.