Notes on quantum transport in mesoscopic systems

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Contents

0.1 Basics

0.1.1 Magnon

A magnon is a quasiparticle, a collective excitation of the electrons' spin structure in a crystal lattice. In the equivalent wave picture of quantum mechanics, a magnon can be viewed as a quantized spin wave. Magnons carry a fixed amount of energy and lattice momentum, and are spin-1, indicating they obey boson behavior.

0.1.2 Hall effect

Conventional Hall effect

Quantum Hall effect

Spin Hall effect

Occurs in paramagnetic systems as a result of spin-orbit interaction, refers to generation of pure spin current transverse to an applied electric field, even in the absence of magnetic field.

Similar to charge accumulation at sample edges in conventional Hall effect, spin accumulation is expected in spin Hall effect.

- extrinsic spin Hall effect: originates from asymmetric scattering for spin-up and spin-down.
- intrinsic spin Hall effect: originates from band structures without scattering.[1]

Fractional Hall effect

Anomalous Hall effect

0.2 Formulas in PRB. 88, 220406(R) (2013)

0.2.1 Formula 1

System Hamiltonion:

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

Left lead is metallic

$$H_L = \sum_{k\sigma} (\varepsilon_{k\sigma} - \mu_\sigma)\, c^\dagger_{k\sigma} c_{k\sigma}, \tag{2}$$

right lead is insulating magnetic

$$H_R \approx \sum_q \hbar w_q a^\dagger_q a_q + \text{ constant } . \tag{3}$$

The interfacial electron-magnon interaction is described by

$$H_{sd} = -\sum_{k,q} J_q \left[S^-_q c^\dagger_{k\uparrow} c_{k+q\downarrow} + S^+_q c^\dagger_{k+q\downarrow} c_{k\uparrow} \right] \tag{4}$$

where $S^-_q \approx \sqrt{2S_0} a^\dagger_q, S^+_q \approx \sqrt{2S_0} a_q$ are in the momentum space and J_q denotes the effective exchange coupling at the interface. The magnonic spin current operator can be obtained by

$$\hat{I}_S = \frac{d\hat{N}_R}{dt} = \frac{d}{dt} \sum_q a^\dagger_q a_q, \tag{5}$$

the magnonic spin current is obtained by taking average over the nonequilibrium ground state $|\psi_0\rangle$ of the interacting system H:

$$I_S = \frac{dN_R}{dt} = \frac{d}{dt} \langle \sum_q a^\dagger_q a_q \rangle. \tag{6}$$

Using the Heisenberg equation, we get

$$I_S = \frac{i}{\hbar}\langle [H_{sd}, \sum_q a_q^\dagger a_q]\rangle. \tag{7}$$

$$[H_{sd}, \sum_q a_q^\dagger a_q] = [-\sum_{k,q} J_q \left(S_q^- c_{k\uparrow}^\dagger c_{k+q\downarrow} + S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right), \sum_q a_q^\dagger a_q], \tag{8}$$

in which,

$$[a_q^\dagger, \sum_{q'} a_{q'}^\dagger, a_{q'}] = \delta_{qq'}[a_q^\dagger, a_{q'}^\dagger a_{q'}] = [a_q^\dagger, a_q^\dagger a_q] = a_q^\dagger[a_q^\dagger, a_q] = -a_q^\dagger. \tag{9}$$

Similarly,

$$[a_q, \sum_{q'} a_{q'}^+ a_{q'}] = [a_q, a_q^\dagger a_q] = a_q. \tag{10}$$

So,

$$\begin{aligned} I_S &= \frac{i}{\hbar}\langle -\sum_{kq} J_q \left(-S_q^- c_{k\uparrow}^\dagger c_{k+q\downarrow} + S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right)\rangle \\ &= \frac{i}{\hbar}\sum_{kq} J_q \left(\langle S_q^- c_{k\uparrow}^\dagger c_{k+q\downarrow}\rangle - \langle S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\rangle\right). \end{aligned} \tag{11}$$

0.2.2 Formula 2

$$\frac{d}{dt}\left\langle S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right\rangle = \frac{i}{\hbar}\left\langle \left[H_L + H_{sd} + H_R, S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right]\right\rangle. \tag{12}$$

The rhs. of eq. (12) is decomposed into 3 terms. The first term reads

$$\begin{aligned} \left\langle \left[H_L, S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right]\right\rangle &= [\sum_{k'\sigma} (\varepsilon_{k'\sigma} - \mu_\sigma)\, c_{k'\sigma}^\dagger c_{k'\sigma}, S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}] \\ &= S_q^+ [\sum_{k'\sigma} (\varepsilon_{k'\sigma} - \mu_\sigma)\, c_{k'\sigma}^\dagger c_{k'\sigma}, c_{k+q\downarrow}^\dagger] c_{k\uparrow} \\ &\quad + S_q^+ c_{k+q\downarrow}^\dagger [\sum_{k'\sigma} (\varepsilon_{k'\sigma} - \mu_\sigma)\, c_{k'\sigma}^\dagger c_{k'\sigma}, c_{k\uparrow}] \end{aligned} \tag{13}$$

Note that,

$$[\sum_{k'\sigma} c_{k'\sigma}^\dagger c_{k'\sigma}, c_{k+q\downarrow}^\dagger] = \sum_{k'\sigma} c_{k'\sigma}^\dagger \delta_{k',k+q}\delta_{\sigma\downarrow} = c_{k+q\downarrow}^\dagger, \tag{14}$$

$$[\sum_{k'\sigma} c_{k'\sigma}^\dagger c_{k'\sigma}, c_{k\uparrow}] = -\sum_{k'\sigma} \{c_{k'\sigma}^\dagger, c_{k\uparrow}\} c_{k'\sigma} = -c_{k\uparrow}. \tag{15}$$

Eq. (14) (15) are derived using equity

$$\begin{aligned} [AB, C] &= A[B, C] + [A, C]B \\ &= A\{B, C\} - \{A, C\}B. \end{aligned} \tag{16}$$

So,

$$\left[H_L, S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right] = (\varepsilon_{k+q\downarrow} - \varepsilon_{k\uparrow} + \mu_\uparrow - \mu_\downarrow)\, S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}. \tag{17}$$

If $\mu_\uparrow = \mu_\downarrow$, then eq. (17) reduces to

$$\left[H_L, S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right] = \left(\varepsilon_{k+q\downarrow} - \varepsilon_{k\uparrow}\right) S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}. \tag{18}$$

The second term $H_R = \sum_q \hbar w_q a_q^\dagger a_q$, then using eq. (10), we get

$$\left[H_R, S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right] = -\hbar\omega_q S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}. \tag{19}$$

The third term in eq. (12) reads

$$\begin{aligned}\left[H_{sd}, S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right] &= -J_q \left[S_q^- c_{k\uparrow}^\dagger c_{k+q\downarrow}, S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right] \\ &= J_q \left[S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}, S_q^- c_{k\uparrow}^\dagger c_{k+q\downarrow}\right]\end{aligned} \tag{20}$$

Combine these three terms, we get

$$\begin{aligned}\frac{d}{dt}\left\langle S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right\rangle &= \frac{i}{\hbar}\left(\varepsilon_{k+q\downarrow} - \varepsilon_{k\uparrow} - \hbar\omega_q\right)\left\langle S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}\right\rangle \\ &+ \frac{i}{\hbar} J_q \left\langle \left[S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow}, S_q^- c_{k\uparrow}^\dagger c_{k+q\downarrow}\right]\right\rangle,\end{aligned} \tag{21}$$

which is also eq. (2) in PRB. 88, 220406(R) (2013).

0.3 Spin current in NM-QD-MIL system

For system consists of quantum dot(QD) sandwiched by a left normal metal(NM) lead and a right magnetic insulating lead(MIL), the Hamiltonian is

$$H = H_{\mathrm{L}} + H_{\mathrm{QD}} + H_{\mathrm{R}} + H_{\mathrm{T}}. \tag{22}$$

$$H_{\mathrm{L}} = \sum_{k\sigma} \varepsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma}, \tag{23}$$

$$H_{\mathrm{QD}} = \sum_{\sigma} \varepsilon_\sigma d_\sigma^\dagger d_\sigma, \tag{24}$$

$$H_{\mathrm{R}} \approx \sum_q \hbar w_q a_q^\dagger a_q, \tag{25}$$

$$H_{\mathrm{T}} = V_{\mathrm{L}} + V_{\mathrm{R}} \tag{26}$$

V$_L$ is the coupling between left lead and QD, while V$_R$ is the coupling between right lead and QD.

$$V_{\mathrm{L}} = \sum_{k\sigma}(t_{k\sigma} c_{k\sigma}^\dagger d_\sigma + t_{k\sigma}^* d_\sigma^\dagger c_{k\sigma}) \tag{27}$$

$$V_{\mathrm{R}} = -\sum_q J_q \left[S_q^- d_\uparrow^\dagger d_\downarrow + S_q^+ d_\downarrow^\dagger d_\uparrow\right]. \tag{28}$$

where $S_q^- \approx \sqrt{2S_0} a_q^\dagger, S_q^+ \approx \sqrt{2S_0} a_q$ are in the momentum space and J_q denotes the effective exchange coupling between the QD and MIL.

0.3.1 Spin-dependent current in left lead

The spin-dependent current flow out of left lead is $I_{L\sigma}$:

$$I_{L\sigma} = \frac{d}{dt}\langle N_{L\sigma}\rangle \tag{29}$$

in which, $N_{L\sigma} = \sum_k c^\dagger_{k\sigma} c_{k\sigma}$ Heisenberg equation:

$$\frac{d}{dt}\langle N_{L\sigma}\rangle = \frac{i}{\hbar}\langle [H, N_{L\sigma}]\rangle \tag{30}$$

$$[H, N_{L\sigma}] = [H_T, N_{L\sigma}] = \sum_k \left(t^*_{k\sigma} d^\dagger_\sigma c_{k\sigma} - t_{k\sigma} c^\dagger_{k\sigma} d_\sigma \right) \tag{31}$$

so, the spin-dependent current

$$I_{L\sigma} = \frac{i}{\hbar}\sum_k \left(t^*_{k\sigma}\langle d^\dagger_\sigma c_{k\sigma}\rangle - t_{k\sigma}\langle c^\dagger_{k\sigma} d_\sigma\rangle \right). \tag{32}$$

Namely, the spin-up current is

$$I_{L\uparrow} = \frac{i}{\hbar}\sum_k \left(t^*_{k\uparrow}\langle d^\dagger_\uparrow c_{k\uparrow}\rangle - t_{k\uparrow}\langle c^\dagger_{k\uparrow} d_\uparrow\rangle \right), \tag{33}$$

the spin-down current is

$$I_{L\downarrow} = \frac{i}{\hbar}\sum_k \left(t^*_{k\downarrow}\langle d^\dagger_\downarrow c_{k\downarrow}\rangle - t_{k\downarrow}\langle c^\dagger_{k\downarrow} d_\downarrow\rangle \right), \tag{34}$$

The charge current in left lead is defined as

$$I_e = e(I_{L\uparrow} + I_{L\downarrow}). \tag{35}$$

The spin current in left lead is defined as

$$I_{LS} = \frac{1}{2}(I_{L\uparrow} - I_{L\downarrow}) \tag{36}$$

Substitute the spin-dependent current in, we get the spin current in left lead

$$I_{LS} = \frac{i}{2\hbar}\sum_k \left(t^*_{k\uparrow}\langle d^\dagger_\uparrow c_{k\uparrow}\rangle - t_{k\uparrow}\langle c^\dagger_{k\uparrow} d_\uparrow\rangle - t^*_{k\downarrow}\langle d^\dagger_\downarrow c_{k\downarrow}\rangle + t_{k\downarrow}\langle c^\dagger_{k\downarrow} d_\downarrow\rangle \right) \tag{37}$$

0.3.2 magnonic current in right lead

The magnonic current in right lead is

$$I_{RS} = \frac{d\langle N_R\rangle}{dt} = \frac{d}{dt}\langle \sum_q a^\dagger_q a_q\rangle, \tag{38}$$

From the Heisenberg equation, we have

$$\frac{d}{dt}\langle\sum_q a_q^\dagger a_q\rangle = \frac{i}{\hbar}\langle[H,\sum_q a_q^\dagger a_q]\rangle. \tag{39}$$

We have

$$\begin{aligned}
&[H,\sum_q a_q^\dagger a_q]\\
=&[V_R,\sum_q a_q^\dagger a_q]\\
=&-\sum_q J_q\Big(\big[S_q^- d_\uparrow^\dagger d_\downarrow,\sum_{q'} a_{q'}^\dagger a_{q'}\big]+\big[S_q^+ d_\downarrow^\dagger d_\uparrow,\sum_{q'} a_{q'}^\dagger a_{q'}\big]\Big)\\
=&\sum_q J_q\big(S_q^- d_\uparrow^\dagger d_\downarrow - S_q^+ d_\downarrow^\dagger d_\uparrow\big)
\end{aligned} \tag{40}$$

So, the magnon current reads

$$I_{RS} = \frac{i}{\hbar}\sum_q J_q\big(\langle S_q^- d_\uparrow^\dagger d_\downarrow\rangle - \langle S_q^+ d_\downarrow^\dagger d_\uparrow\rangle\big). \tag{41}$$

0.3.3 spin-dependent current in QD

Similarly, the spin-dependent current in the central QD is defined as

$$I_{C\sigma} = \langle\frac{dN_{C\sigma}}{dt}\rangle = \langle\frac{d}{dt}d_\sigma^\dagger d_\sigma\rangle, \tag{42}$$

Heisenberg equation:

$$\frac{d}{dt}d_\sigma^\dagger d_\sigma = \frac{i}{\hbar}[H,d_\sigma^\dagger d_\sigma]. \tag{43}$$

Specifically, we have

$$[H,d_\sigma^\dagger d_\sigma] = [V_L,d_\sigma^\dagger d_\sigma] + [V_R,d_\sigma^\dagger d_\sigma] \tag{44}$$

in which,

$$\begin{aligned}
[V_L,d_\sigma^\dagger d_\sigma] &= \sum_{k'\sigma'}\big(t_{k'\sigma'}\big[c_{k'\sigma'}^\dagger d_{\sigma'},d_\sigma^\dagger d_\sigma\big] + t_{k'\sigma'}^*\big[d_{\sigma'}^\dagger c_{k'\sigma'},d_\sigma^\dagger d_\sigma\big]\big)\\
&= \sum_{k'\sigma'}\big(t_{k'\sigma'}c_{k'\sigma'}^\dagger d_{\sigma'}\delta_{\sigma\sigma'} - t_{k'\sigma'}^* d_{\sigma'}^\dagger c_{k'\sigma'}\delta_{\sigma\sigma'}\big)\\
&= \sum_k\big(t_{k\sigma}c_{k\sigma}^\dagger d_\sigma - t_{k\sigma}^* d_\sigma^\dagger c_{k\sigma}\big)
\end{aligned} \tag{45}$$

We change the summation index from k' to k in the last line , which doesn't change the result.

$$[V_R,d_\sigma^\dagger d_\sigma] = -\sum_q J_q\big(S_q^-\big[d_\uparrow^\dagger d_\downarrow,d_\sigma^\dagger d_\sigma\big] + S_q^+\big[d_\downarrow^\dagger d_\uparrow,d_\sigma^\dagger d_\sigma\big]\big) \tag{46}$$

in which,

$$\begin{aligned}
\big[d_\uparrow^\dagger d_\downarrow,d_\sigma^\dagger d_\sigma\big] &= d_\uparrow^\dagger\big[d_\downarrow,d_\sigma^\dagger d_\sigma\big] + \big[d_\uparrow^\dagger,d_\sigma^\dagger d_\sigma\big]d_\downarrow\\
&= d_\uparrow^\dagger d_\downarrow\delta_{\sigma\downarrow} - d_\uparrow^\dagger d_\downarrow\delta_{\sigma\uparrow}
\end{aligned} \tag{47}$$

So,

$$[V_R, d_\sigma^\dagger d_\sigma] = -\sum_q J_q \big[S_q^- \left(d_\uparrow^\dagger d_\downarrow \delta_{\sigma\downarrow} - d_\uparrow^\dagger d_\downarrow \delta_{\sigma\uparrow}\right) + S_q^+ \left(d_\downarrow^\dagger d_\uparrow \delta_{\sigma\uparrow} - d_\downarrow^\dagger d_\uparrow \delta_{\sigma\downarrow}\right)\big] \tag{48}$$

The spin-dependent current is

$$I_{C\uparrow} = \frac{i}{\hbar}\big[H, d_\uparrow^\dagger d_\uparrow\big] \tag{49}$$

$$I_{C\downarrow} = \frac{i}{\hbar}\big[H, d_\downarrow^\dagger d_\downarrow\big] \tag{50}$$

which gives

$$I_{C\uparrow} = \frac{i}{\hbar}\big[\sum_k \left(t_{k\uparrow} c_{k\uparrow}^\dagger d_\uparrow - t_{k\uparrow}^* d_\uparrow^\dagger c_{k\uparrow}\right) + \sum_q J_q \big(S_q^- d_\uparrow^\dagger d_\downarrow - S_q^+ d_\downarrow^\dagger d_\uparrow\big)\big] \tag{51}$$

and

$$I_{C\downarrow} = \frac{i}{\hbar}\big[\sum_k \left(t_{k\downarrow} c_{k\downarrow}^\dagger d_\downarrow - t_{k\downarrow}^* d_\downarrow^\dagger c_{k\downarrow}\right) + \sum_q J_q \big(S_q^+ d_\downarrow^\dagger d_\uparrow - S_q^- d_\uparrow^\dagger d_\downarrow\big)\big]. \tag{52}$$

The spin current in central dot is

$$I_{CS} = \frac{1}{2}(I_{C\uparrow} - I_{C\downarrow}) \tag{53}$$

0.3.4 Verifying continuity condition

Charge current

Since the right lead is a insulating lead, there is no charge current flow through it, so the charge current is

$$I_{Re} = 0 \tag{54}$$

where the subscript R denotes the right lead, while the subscript e denotes the charge current.

Meanwhile, the charge current flows in left lead and QD is

$$I_e = e\big(\sum_\sigma I_{L\sigma} + \sum_\sigma I_{C\sigma}\big) = 0 \tag{55}$$

Spin current

Spin current in the left lead and QD:

$$I_{LS} + I_{CS} = \frac{i}{\hbar}\sum_q J_q \big(\langle S_q^- d_\uparrow^\dagger d_\downarrow\rangle - \langle S_q^+ d_\downarrow^\dagger d_\uparrow\rangle\big). \tag{56}$$

The magnon current is

$$I_{RS} = \frac{i}{\hbar}\sum_q J_q \big(\langle S_q^- d_\uparrow^\dagger d_\downarrow\rangle - \langle S_q^+ d_\downarrow^\dagger d_\uparrow\rangle\big), \tag{57}$$

in which, I_{LS}, I_{CS}, I_{RS} is defined earlier. Thus, we have

$$\begin{aligned} I_{LS} + I_{CS} &= I_{RS} \\ &= \frac{i}{\hbar}\sum_q J_q \big(\langle S_q^- d_\uparrow^\dagger d_\downarrow\rangle - \langle S_q^+ d_\downarrow^\dagger d_\uparrow\rangle\big). \end{aligned} \tag{58}$$

0.3.5 Perturbation expansion of $G_d(\tau, \tau)$

When neglecting left lead, the hamiltonian is

$$H = H_{QD} + H_R + H_{sd} \tag{59}$$

Expand S-matrix up to the second order of J, we have

$$\begin{aligned}
&G_d(\tau, \tau) = -i\langle T_C S s_q^+(\tau) s_q^-(\tau')\rangle \\
=& -i\sum_k g_{k\uparrow}(\tau', \tau) g_{k+q\downarrow}(\tau, \tau') \\
&+ \int_c d\tau_1 \int_c d\tau_2 \sum_{kq_1} J_{q_1}^2 g_{Rq_1}(\tau_2, \tau_1) g_{k\uparrow}(\tau', \tau_2) g_{k+q_1\downarrow}(\tau_2, \tau_1) g_{k\uparrow}(\tau_1, \tau) g_{k+q\downarrow}(\tau, \tau') \\
&+ \int_c d\tau_1 \int_c d\tau_2 \sum_{kq_1} J_{q_1}^2 g_{Rq_1}(\tau_2, \tau_1) g_{k\uparrow}(\tau', \tau) g_{k+q\downarrow}(\tau, \tau_1) g_{k+q-q_1\uparrow}(\tau_1, \tau_2) g_{k+q\downarrow}(\tau_2, \tau') \\
&- \int_c d\tau_1 \int_c d\tau_2 \sum_{kk'} J_q^2 g_{Rq}(\tau_2, \tau_1) g_{k\uparrow}(\tau_1, \tau) g_{k+q\downarrow}(\tau, \tau_1) g_{k'\uparrow}(\tau', \tau_2) g_{k'+q\downarrow}(\tau_2, \tau')
\end{aligned} \tag{60}$$

0.4 Checking formulas in notes

0.5 Nonequilibrium Green's function technique

0.5.1 Demonstrative Hamiltonian

$$\hat{H} = H_{lead} + H_{dot} + H_T \tag{61}$$

$$H_{lead} = \sum_{k\alpha} \epsilon_{k\alpha} \hat{C}_{k\alpha}^\dagger \hat{C}_{k\alpha} \tag{62}$$

$$\epsilon_{k\alpha} = \epsilon_{k\alpha}^{(0)} + qv_\alpha \tag{63}$$

$$H_{dot} = \sum_n (\epsilon_n + qU_n)\, d_n^\dagger d_n \tag{64}$$

$$U_n = \sum_m V_{nm} < d_m^\dagger d_m > \tag{65}$$

$$H_T = \sum_{k\alpha n} \left[t_{k\alpha n} \hat{C}_{k\alpha}^\dagger \hat{d}_n + t_{k\alpha n}^* \hat{d}_n^\dagger \hat{C}_{k\alpha} \right] \tag{66}$$

0.5.2 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

$$\begin{aligned}\frac{d}{dt}\hat{N}_\alpha &= \frac{i}{\hbar}[H, \sum_k c^\dagger_{\alpha k} c_{\alpha k}] = \left[\sum_{k'n,\alpha'=L,R}\left[t_{k'\alpha'} c^\dagger_{k'\alpha'} d_n + \text{c.c.}\right], \sum_k c^\dagger_{\alpha k} c_{\alpha k}\right] \\ &= \frac{i}{\hbar}\sum_{kk',n,\alpha'=L,R}\left[-t_{k'\alpha'} c^\dagger_{k'\alpha'} d_n \delta_{\alpha\alpha'}\delta_{kk'} + \text{c.c.}\right] \\ &= \frac{i}{\hbar}\sum_{kn}[-t_{k\alpha} c^\dagger_{k\alpha} d_n + t^*_{k\alpha} d^\dagger_n c_{k\alpha}]\end{aligned} \tag{67}$$

So, the charge current is given by

$$\begin{aligned}I_\alpha(t) &= e\langle\frac{d}{dt}\hat{N}_\alpha(t)\rangle \\ &= \frac{ie}{\hbar}\sum_{kn}(\langle -t_{k\alpha} c^\dagger_{k\alpha}(t) d_n(t)\rangle + \langle t^*_{k\alpha} d^\dagger_n(t) c_{k\alpha}(t)\rangle)\end{aligned} \tag{68}$$

Define the lesser Green's function

$$G^<_{\sigma',k\alpha\sigma}(t,t') = i\langle c^\dagger_{k\alpha\sigma}(t') d_{\sigma'}(t)\rangle \tag{69}$$

the charge current is written as

$$I_L(t) = \frac{-e}{\hbar}\sum_{kn\alpha\in L}(t_{k\alpha n} G^<_{n,k\alpha\sigma}(t,t) - t^*_{k\alpha n} G_{k\alpha,n}(t,t)\rangle) \tag{70}$$

More generally, we define the contour Green's function

$$G_{n,k\alpha}(\tau,\tau') = -i\langle d_n(\tau) c^\dagger_{k\alpha}(\tau')\rangle. \tag{71}$$

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

$$G_{n,k\alpha}(\tau,\tau') = \sum_m \int d\tau_1 G_{nm}(\tau,\tau_1)\, t^*_{k\alpha m} g_{k\alpha}(\tau_1,\tau') \tag{72}$$

where

$$G_{nm}(\tau_1,\tau_2) \equiv -i\langle T_c\left[d_n(\tau_1)\, d^\dagger_m(\tau_2)\right]\rangle \tag{73}$$

$$g_{k\alpha}(\tau_1,\tau_2) \equiv -i\langle T_c\left[c_{k\alpha}(\tau_1)\, c^\dagger_{k\alpha}(\tau_2)\right]\rangle_0. \tag{74}$$

Using the theorem of analytic continuation, we have

$$\begin{aligned}G^<_{n,k\alpha}(t,t') = \sum_m \int dt_1 &\left[G^r_{nm}(t,t_1)\, t^*_{k\alpha m} g^<_{k\alpha}(t_1,t')\right. \\ &\left.+ G^<_{nm}(t,t_1)\, t^*_{k\alpha m} g^a_{k\alpha}(t_1,t')\right].\end{aligned} \tag{75}$$

This gives the term in current

$$\begin{aligned}
&\sum_{kn} t_{k\alpha n} G^{<}_{n,k\alpha}\left(t,t'\right) = \sum_{kmn} \int dt_1 t_{k\alpha n} t^{*}_{k\alpha m} \\
&\times \left[G^{r}_{nm}\left(t,t_1\right) g^{<}_{k\alpha}\left(t_1,t'\right) + G^{<}_{nm}\left(t,t_1\right) g^{a}_{k\alpha}\left(t_1,t'\right)\right] \\
&= \sum_{n} \int dt_1 \left[G^{r}\left(t,t_1\right) \Sigma^{<}_{\alpha}\left(t_1,t'\right) + G^{<}\left(t,t_1\right) \Sigma^{a}_{\alpha}\left(t_1,t'\right)\right]_{nn}
\end{aligned} \tag{76}$$

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

$$\Sigma^{\gamma}_{\alpha,mn}(t_1,t_2) = \sum_k t^{*}_{k\alpha m}(t_1) g^{\gamma}_{k\alpha}(t_1,t_2) t_{k\alpha n}(t_2). \tag{77}$$

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

$$\begin{aligned}
I_\alpha(t) = -\frac{e}{\hbar} \int dt_1 \operatorname{Tr} \big[& G^{r}\left(t,t_1\right) \Sigma^{<}_{\alpha}\left(t_1,t\right) \\
&+ G^{<}\left(t,t_1\right) \Sigma^{a}_{\alpha}\left(t_1,t\right) \big] + h.c.
\end{aligned} \tag{78}$$

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.

0.5.3 Free propagators

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

$$g^{<}_{k\sigma}\left(t,t'\right) \equiv i \left\langle c^{\dagger}_{k\sigma}\left(t'\right) c_{k\sigma}(t) \right\rangle = i f(\varepsilon^{(0)}_{k}) e^{-i\int_{t'}^{t} dt_1 \varepsilon_{k\sigma}(t_1)} \tag{79}$$

$$g^{>}_{k\sigma}\left(t,t'\right) \equiv -i \left\langle c_{k\sigma}(t) c^{\dagger}_{k\sigma}\left(t'\right) \right\rangle = i \left[f\left(\varepsilon_k\right) - 1\right] e^{-i\varepsilon_{k\sigma}(t-t')} \tag{80}$$

$$g^{r}_{k\sigma}(t) \equiv -i\theta(t) \left\langle \left[c_{k\sigma}(t), c^{\dagger}_{k\sigma}\left(t'\right)\right]_{+} \right\rangle = -i\theta(t) e^{-i\varepsilon_{k\sigma}(t-t')} \tag{81}$$

$$g^{a}_{k\sigma}(t) \equiv i\theta(-t) \left\langle \left[c_{k\sigma}(t), c^{\dagger}_{k\sigma}\left(t'\right)\right]_{+} \right\rangle = i\theta(-t) e^{-i\varepsilon_{k\sigma}(t-t')} \tag{82}$$

Using the relation

$$\int dt e^{i\omega t} = 2\pi\delta(\omega), \tag{83}$$

Fourier transformation gives

$$g^{<}_{k\sigma}(\omega) = 2\pi i f\left(\varepsilon_{k\sigma}\right) \delta\left(\omega - \varepsilon_{k\sigma}\right) = i f\left(\varepsilon_{k\sigma}\right) A_0(k,\omega) \tag{84}$$

$$g^{>}_{k\sigma}(\omega) = 2\pi i \left[f\left(\varepsilon_{k\sigma}\right) - 1\right] \delta\left(\omega - \varepsilon_{k\sigma}\right) \tag{85}$$

$$g^{r}_{k\sigma}(\omega) = -i \int_{-\infty}^{\infty} dt e^{i\omega t} \theta(t) e^{-i\epsilon_{k\sigma} t} = -i \int_{0}^{\infty} dt e^{i(\omega - \epsilon_{k\sigma})t} = \frac{-i}{i(\omega - \varepsilon_{k\sigma})} e^{i(\omega-\varepsilon)}|_{0}^{+\infty} \tag{86}$$

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

$$g^{r}_{k\sigma}(\omega) = \frac{1}{\omega - \varepsilon_{k\sigma} + i0^{+}}. \tag{87}$$

Similarly,

$$g^a_{k\sigma}(\omega) = \frac{1}{\omega - \varepsilon_{k\sigma} - i0^+}. \tag{88}$$

Then we have

$$g^r_{k\sigma}(\omega) - g^a_{k\sigma}(\omega) = -2\pi i \delta(\omega - \varepsilon_{k\sigma}) \tag{89}$$

The fermion spectral function is defined as

$$\begin{aligned} A_0(k\sigma, \omega) &= i \left[g^r_{k\sigma}(\omega) - g^a_{k\sigma}(\omega)\right] \\ &= -2\Im\text{m}\left[g^r_{k\sigma}(\omega)\right] \\ &= 2\pi\delta\left(\omega - \varepsilon_{k\sigma}\right) \end{aligned} \tag{90}$$

where the following relation are used

$$\frac{1}{x \pm i\eta} = P\frac{1}{x} \mp i\pi\delta(x), \quad \eta = 0^+, \tag{91}$$

$$\Im\text{m}\left[g^r_{k\sigma}(\omega)\right] = -\pi\delta(\omega - \varepsilon_k). \tag{92}$$

0.5.4 DC case

$$G^\gamma\left(t, t_1\right) = G^\gamma\left(t - t_1\right) \tag{93}$$

and

$$\Sigma^\gamma\left(t, t_1\right) = \Sigma^\gamma\left(t - t_1\right) \tag{94}$$

where

$$\gamma = <, >, r, a. \tag{95}$$

Recall that

$$\left[G^<\right]^\dagger(E) = -G^<(E) \tag{96}$$

$$\left[G^r\right]^\dagger = G^a \tag{97}$$

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

$$\begin{aligned} I_\alpha = -\frac{e}{\hbar}\int \frac{dE}{2\pi}\,\text{Tr}\,&\big[\left(G^r(E) - G^a(E)\right)\Sigma^<_\alpha(E) \\ &+G^<(E)\left(\Sigma^a_\alpha(E) - \Sigma^r_\alpha(E)\right)\big] \end{aligned} \tag{98}$$

Substitute free propagators in, we have

$$\Sigma^<_{\alpha,mn}(t-t_1) = \sum_k t^*_{k\alpha m}(t_1) g^<_{k\alpha}(t_1 - t_2) t_{k\alpha n}(t_2) = i\sum_k t^*_{k\alpha m}(t_1) f(\epsilon_{k\alpha}) e^{-i\varepsilon_{k\alpha(t-t_1)}} t_{k\alpha n}(t_2) \tag{99}$$

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

$$\Sigma^<_{\alpha,mn}(E) = 2\pi i \sum_k t^*_{k\alpha m} f(\varepsilon_{k\alpha}) t_{k\alpha n}\delta(E - \varepsilon_{k\alpha}) \tag{100}$$

$$\Sigma^a_\alpha(E) - \Sigma^r_\alpha(E) = \sum_k t^*_{k\alpha m}(g^a_{k\alpha}(E) - g^r_{k\alpha}(E)) t_{k\alpha n} \tag{101}$$

which according to Eq. (89), we have

$$\Sigma_{\alpha}^{a}(E)-\Sigma_{\alpha}^{r}(E)=2\pi i\sum_{k}t_{k\alpha m}^{*}\delta(E-\epsilon_{k\alpha})t_{k\alpha n}. \tag{102}$$

Define a level-width function:

$$\Gamma_{\alpha,mn}(E)=\sum_{k}2\pi t_{k\alpha m}^{*}t_{k\alpha n}\delta\left(E-\varepsilon_{k\alpha}\right) \tag{103}$$

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

$$\Sigma_{\alpha,mn}^{<}(E)=if(\varepsilon_{k\alpha})\Gamma_{\alpha,mn}(E) \tag{104}$$

and

$$\Sigma_{\alpha}^{a}(E)-\Sigma_{\alpha}^{r}(E)=i\Gamma_{\alpha,mn}(E) \tag{105}$$

Then Eq. (98) can be written as

$$\begin{aligned}I_{\alpha}=&-\frac{e}{\hbar}\int\frac{dE}{2\pi}\operatorname{Tr}\left[\left(G^{r}(E)-G^{a}(E)\right)\left(if(\varepsilon_{k\alpha}\Gamma_{\alpha,mn}(E))\right)\right.\\&\left.+G^{<}(E)(i\Gamma_{\alpha,mn}(E))\right)\\=&-\frac{ie}{\hbar}\int\frac{dE}{2\pi}\operatorname{Tr}\left[\Gamma_{\alpha,mn}(E)(\left[G^{r}(E)-G^{a}(E)\right]f(\varepsilon_{k\alpha})+G^{<}(E))\right]\end{aligned} \tag{106}$$

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

$$\begin{aligned}I=-\frac{\mathrm{i}e}{2\hbar}\int\frac{\mathrm{d}\varepsilon}{2\pi}\operatorname{Tr}&\left\{\left[\mathbf{\Gamma}^{L}(\varepsilon)-\mathbf{\Gamma}^{R}(\varepsilon)\right]\mathbf{G}^{<}(\varepsilon)\right.\\&\left.+\left[f_{L}(\varepsilon)\mathbf{\Gamma}^{L}(\varepsilon)-f_{R}(\varepsilon)\mathbf{\Gamma}^{R}(\varepsilon)\right]\left[\mathbf{G}^{\mathrm{r}}(\varepsilon)-\mathbf{G}^{\mathrm{a}}(\varepsilon)\right]\right\}\end{aligned} \tag{107}$$

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

$$\mathbf{\Gamma}^{L}(\varepsilon)=\lambda\mathbf{\Gamma}^{R}(\varepsilon) \tag{108}$$

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

$$\begin{aligned}J&=\frac{1e}{\hbar}\int\frac{\mathrm{d}\varepsilon}{2\pi}\left[f_{L}(\varepsilon)-f_{R}(\varepsilon)\right]\mathcal{T}(\varepsilon)\\\mathcal{T}(\varepsilon)&=\operatorname{Tr}\left\{\frac{\Gamma^{L}(\varepsilon)\Gamma^{R}(\varepsilon)}{\Gamma^{L}(\varepsilon)+\Gamma^{R}(\varepsilon)}\left[\mathbf{G}^{\mathrm{r}}(\varepsilon)-\mathbf{G}^{\mathrm{a}}(\varepsilon)\right]\right\}\end{aligned} \tag{109}$$

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 $T(\varepsilon)$.

0.5.5 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

$$G = G_0 + G_0 \Sigma G \tag{110}$$

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

$$G^{<,>} = G_0^{<,>} + G^r \Sigma^r G_0^{<,>} + G^{<,>} \Sigma^a G_0^a + G^r \Sigma^{<,>} G_0^a \tag{111}$$

or

$$G^{<,>} = G_0^{<,>} + G_0^r \Sigma^r G^{<,>} + G_0^{<,>} \Sigma^a G^a + G_0^r \Sigma^{<,>} G^a \tag{112}$$

or

$$G^{<} = G^r \left(G_0^r\right)^{-1} G_0^{<} \left(G_0^a\right)^{-1} G^a + G^r \Sigma^{<} G^a \tag{113}$$

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

0.5.6 With spin index

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

$$\begin{aligned} I_{\beta\sigma} = \tfrac{e}{h} \textstyle\sum_{k,i,j} \int d\omega V_{ki\beta\sigma} V^*_{kj\beta\sigma} \Big\{ & \Big[G^r_{i\sigma,j\sigma}(\omega) - G^a_{i\sigma,j\sigma}(\omega) \Big] g^<_{k\beta\sigma}(\omega) \\ & - \Big[g^r_{k\beta\sigma}(\omega) - g^a_{k\beta\sigma}(\omega) \Big] G^<_{i\sigma,j\sigma}(\omega) \Big\}. \end{aligned} \tag{114}$$

Substitute free propagators into current formula, we have

$$I_{\beta\sigma} = \frac{ie}{h} \sum_{i,j} \int d\omega \Gamma_{ij\beta\sigma}(\omega) \left\{ \left[G^r_{i\sigma,j\sigma}(\omega) - G^a_{i\sigma,j\sigma}(\omega) \right] f_\beta(\omega) + G^<_{i\sigma,j\sigma}(\omega) \right\} \tag{115}$$

self-energy of lead α is

$$\Sigma^<_\alpha(\omega) = i\Gamma_\alpha\left(\omega - qv_\alpha\right) f_\alpha(\omega) \tag{116}$$

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