Notes on quantum transport in mesoscopic systems

Li Gaoyang

October 17, 2020

# Contents

0.1	Basics	3
	0.1.1 Magnon	3
	0.1.2 Hall effect	3
0.2	Formulas in PRB. 88, 220406(R) (2013)	4
	0.2.1 Formula 1	4
	0.2.2 Formula 2	5
0.3	Spin current in NM-QD-MIL system	6
	0.3.1 Spin-dependent current in left lead	6
	0.3.2 magnonic current in right lead	7
	0.3.3 spin-dependent current in QD	7
	0.3.4 Verifying continuity condition	8
	0.3.5 Perturbation expansion of $G_d(\tau,\tau)$	
	0.3.6 new hamiltonian	9
	0.3.7 Calculation of $G_d$	10
	0.3.8 continuation on Eq.(88)	11
0.4	Nonequilibrium Green's function technique	12

#### 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:

$$H = H_L + H_R + H_{sd}. (1)$$

Left lead is metallic

$$H_L = \sum_{k\sigma} \left( \varepsilon_{k\sigma} - \mu_{\sigma} \right) c_{k\sigma}^{\dagger} c_{k\sigma}, \tag{2}$$

right lead is insulating magnetic

$$H_R \approx \sum_q \hbar w_q a_q^{\dagger} a_q + \text{ constant }.$$
 (3)

The interfacial electron-magnon interaction is described by

$$H_{sd} = -\sum_{k,q} J_q \left[ S_q^- c_{k\uparrow}^\dagger c_{k+q\downarrow} + S_q^+ c_{k+q\downarrow}^\dagger c_{k\uparrow} \right]$$
 (4)

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 at the interface. The magnonic spin current operator can be obtained by

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

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

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

Using the Heisenberg equation, we get

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

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

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,

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

So,

$$I_{S} = \frac{i}{\hbar} \langle -\sum_{kq} J_{q} \left( -S_{q}^{-} c_{k\uparrow}^{\dagger} c_{k+q\downarrow} + S_{q}^{+} c_{k+q\downarrow}^{\dagger} c_{k\uparrow} \right) \rangle$$

$$= \frac{i}{\hbar} \sum_{kq} J_{q} \left( \langle S_{q}^{-} c_{k\uparrow}^{\dagger} c_{k+q\downarrow} \rangle - \langle S_{q}^{+} c_{k+q\downarrow}^{\dagger} c_{k\uparrow} \rangle \right).$$
(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

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

$$= S_q^+ \left[ \sum_{k'\sigma} \left( \varepsilon_{k'\sigma} - \mu_\sigma \right) c_{k'\sigma}^\dagger c_{k'\sigma}, c_{k'\sigma}^\dagger, c_{k+q\downarrow}^\dagger \right] c_{k\uparrow}$$

$$+ S_q^+ c_{k+q\downarrow}^\dagger \left[ \sum_{k'\sigma} \left( \varepsilon_{k'\sigma} - \mu_\sigma \right) c_{k'\sigma}^\dagger c_{k'\sigma}, c_{k\uparrow} \right]$$

$$(13)$$

Note that,

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

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

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

$$[AB, C] = A[B, C] + [A, C]B$$
  
=  $A\{B, C\} - \{A, C\}B$ . (16)

So,

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

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

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

Combine these three terms, we get

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

$$H = H_{\rm L} + H_{\rm QD} + H_{\rm R} + H_{\rm T}.$$
 (22)

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

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

$$H_{\rm R} \approx \sum_{q} \hbar w_q a_q^{\dagger} a_q,$$
 (25)

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

 $V_L$  is the coupling between left lead and QD, while  $V_R$  is the coupling between right lead and QD.

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

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

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:

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

$$[H, N_{L\sigma}] = [H_T, N_{L\sigma}] = \sum_{k} \left( t_{k\sigma}^* d_{\sigma}^{\dagger} c_{k\sigma} - t_{k\sigma} c_{k\sigma}^{\dagger} d_{\sigma} \right)$$
(31)

so, the spin-dependent current

$$I_{L\sigma} = \frac{i}{\hbar} \sum_{k} \left( t_{k\sigma}^* \langle d_{\sigma}^{\dagger} c_{k\sigma} \rangle - t_{k\sigma} \langle c_{k\sigma}^{\dagger} d_{\sigma} \rangle \right). \tag{32}$$

Namely, the spin-up current is

$$I_{L\uparrow} = \frac{i}{\hbar} \sum_{k} \left( t_{k\uparrow}^* \langle d_{\uparrow}^{\dagger} c_{k\uparrow} \rangle - t_{k\uparrow} \langle c_{k\uparrow}^{\dagger} d_{\uparrow} \rangle \right), \tag{33}$$

the spin-down current is

$$I_{L\downarrow} = \frac{i}{\hbar} \sum_{k} \left( t_{k\downarrow}^* \langle d_{\downarrow}^{\dagger} c_{k\downarrow} \rangle - t_{k\downarrow} \langle c_{k\downarrow}^{\dagger} d_{\downarrow} \rangle \right), \tag{34}$$

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

$$I_{LS} = \frac{i}{2\hbar} \sum_{k} \left( t_{k\uparrow}^* \langle d_{\uparrow}^{\dagger} c_{k\uparrow} \rangle - t_{k\uparrow} \langle c_{k\uparrow}^{\dagger} d_{\uparrow} \rangle - t_{k\downarrow}^* \langle d_{\downarrow}^{\dagger} c_{k\downarrow} \rangle + t_{k\downarrow} \langle c_{k\downarrow}^{\dagger} d_{\downarrow} \rangle \right)$$
(37)

#### 0.3.2 magnonic current in right lead

The magnonic current in right lead is

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

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

$$[H, \sum_{q} a_{q}^{\dagger} a_{q}]$$

$$= [V_{R}, \sum_{q} a_{q}^{\dagger} a_{q}]$$

$$= -\sum_{q} J_{q} \left( \left[ S_{q}^{-} d_{\uparrow}^{\dagger} d_{\downarrow}, \sum_{q'} a_{q'}^{\dagger} a_{q'} \right] + \left[ S_{q}^{+} d_{\downarrow}^{\dagger} d_{\uparrow}, \sum_{q'} a_{q'}^{\dagger} a_{q'} \right] \right)$$

$$= \sum_{q} J_{q} \left( S_{q}^{-} d_{\uparrow}^{\dagger} d_{\downarrow} - S_{q}^{+} d_{\downarrow}^{\dagger} d_{\uparrow} \right)$$

$$(40)$$

So, the magnon current reads

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

#### 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,

$$[V_{L}, d_{\sigma}^{\dagger} d_{\sigma}] = \sum_{k'\sigma'} \left( t_{k'\sigma'} \left[ c_{k'\sigma'}^{\dagger} d_{\sigma'}, d_{\sigma}^{\dagger} d_{\sigma} \right] + t_{k'\sigma'}^{*} \left[ d_{\sigma'}^{\dagger} c_{k'\sigma'}, d_{\sigma}^{\dagger} d_{\sigma} \right] \right)$$

$$= \sum_{k'\sigma'} \left( t_{k'\sigma'} c_{k'\sigma'}^{\dagger} d_{\sigma'} \delta_{\sigma\sigma'} - t_{k'\sigma'}^{*} d_{\sigma'}^{\dagger} c_{k'\sigma'} \delta_{\sigma\sigma'} \right)$$

$$= \sum_{k} \left( t_{k\sigma} c_{k\sigma}^{\dagger} d_{\sigma} - t_{k\sigma}^{*} d_{\sigma}^{\dagger} c_{k\sigma} \right)$$

$$(45)$$

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

$$[V_R, d_{\sigma}^{\dagger} d_{\sigma}] = -\sum_{q} J_q \left( S_q^- \left[ d_{\uparrow}^{\dagger} d_{\downarrow}, d_{\sigma}^{\dagger} d_{\sigma} \right] + S_q^+ \left[ d_{\downarrow}^{\dagger} d_{\uparrow}, d_{\sigma}^{\dagger} d_{\sigma} \right] \right)$$

$$\tag{46}$$

in which,

$$\begin{aligned}
 \left[ d_{\uparrow}^{\dagger} d_{\downarrow}, d_{\sigma}^{\dagger} d_{\sigma} \right] &= d_{\uparrow}^{\dagger} \left[ d_{\downarrow}, d_{\sigma}^{\dagger} d_{\sigma} \right] + \left[ d_{\uparrow}^{\dagger}, d_{\sigma}^{\dagger} d_{\sigma} \right] d_{\downarrow} \\
 &= d_{\uparrow}^{\dagger} d_{\downarrow} \delta_{\sigma \downarrow} - d_{\uparrow}^{\dagger} d_{\downarrow} \delta_{\sigma \uparrow}
\end{aligned} (47)$$

So,

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

The spin-dependent current is

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

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

which gives

$$I_{C\uparrow} = \frac{i}{\hbar} \left[ \sum_{k} \left( t_{k\uparrow} c_{k\uparrow}^{\dagger} d_{\uparrow} - t_{k\uparrow}^{*} d_{\uparrow}^{\dagger} c_{k\uparrow} \right) + \sum_{q} J_{q} \left( S_{q}^{-} d_{\uparrow}^{\dagger} d_{\downarrow} - S_{q}^{+} d_{\downarrow}^{\dagger} d_{\uparrow} \right) \right]$$
 (51)

and

$$I_{C\downarrow} = \frac{i}{\hbar} \left[ \sum_{k} \left( t_{k\downarrow} c_{k\downarrow}^{\dagger} d_{\downarrow} - t_{k\downarrow}^{*} d_{\downarrow}^{\dagger} c_{k\downarrow} \right) + \sum_{q} J_{q} \left( S_{q}^{+} d_{\downarrow}^{\dagger} d_{\uparrow} - S_{q}^{-} d_{\uparrow}^{\dagger} d_{\downarrow} \right) \right]. \tag{52}$$

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

$$I_{Re} = 0 (54)$$

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

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

#### Spin current

Spin current in the left lead and QD:

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

The magnon current is

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

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

$$I_{LS} + I_{CS} = I_{RS}$$

$$= \frac{i}{\hbar} \sum_{q} J_q (\langle S_q^- d_{\uparrow}^{\dagger} d_{\downarrow} \rangle - \langle S_q^+ d_{\downarrow}^{\dagger} d_{\uparrow} \rangle).$$
(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

$$G_{d}(\tau,\tau) = -i\langle T_{C}Ss_{q}^{+}(\tau)s_{q}^{-}(\tau')\rangle$$

$$= -i\sum_{k} g_{k\uparrow}(\tau',\tau)g_{k+q\downarrow}(\tau,\tau')$$

$$+ \int_{c} d\tau_{1} \int_{c} d\tau_{2} \sum_{kq_{1}} J_{q_{1}}^{2}g_{Rq_{1}}(\tau_{2},\tau_{1})g_{k\uparrow}(\tau',\tau_{2})g_{k+q_{1}\downarrow}(\tau_{2},\tau_{1})g_{k\uparrow}(\tau_{1},\tau)g_{k+q\downarrow}(\tau,\tau')$$

$$+ \int_{c} d\tau_{1} \int_{c} d\tau_{2} \sum_{kq_{1}} J_{q_{1}}^{2}g_{Rq_{1}}(\tau_{2},\tau_{1})g_{k\uparrow}(\tau',\tau)g_{k+q\downarrow}(\tau,\tau_{1})g_{k+q-q_{1}\uparrow}(\tau_{1},\tau_{2})g_{k+q\downarrow}(\tau_{2},\tau')$$

$$- \int_{c} d\tau_{1} \int_{c} d\tau_{2} \sum_{kk'} J_{q}^{2}g_{Rq}(\tau_{2},\tau_{1})g_{k\uparrow}(\tau_{1},\tau)g_{k+q\downarrow}(\tau,\tau_{1})g_{k'\uparrow}(\tau',\tau_{2})g_{k'+q\downarrow}(\tau_{2},\tau')$$

$$(60)$$

#### 0.3.6 new hamiltonian

$$H = H_L + H_R + H_d + H_T + H_{sd} (61)$$

$$H_L = \sum_{k\sigma} \epsilon_{k\sigma,L} c_{k\sigma}^{\dagger} c_{k\sigma} \tag{62}$$

$$H_R = \sum_q \omega_q a_q^{\dagger} a_q \tag{63}$$

$$H_d = \sum_{n\sigma} \epsilon_{n\sigma} d^{\dagger}_{n\sigma} d_{n\sigma} \tag{64}$$

$$H_T = \sum_{k\sigma n} \left( t_{k\sigma n} c_{k\sigma}^{\dagger} d_{n\sigma} + t_{k\sigma n}^* d_{n\sigma}^{\dagger} c_{k\sigma} \right) \tag{65}$$

$$H_{sd} = -\sum_{qnm} J_q \left( d_{n\uparrow}^{\dagger} d_{m\downarrow} a_q^{\dagger} + a_q d_{m\downarrow}^{\dagger} d_{n\uparrow} \right) \delta \left( \epsilon_{n\uparrow} - \epsilon_{m\downarrow} - \omega_q \right)$$
 (66)

$$s_q^+ = \sum_{nm} d_{n\uparrow}^{\dagger} d_{m\downarrow} \delta_{\uparrow\downarrow} \tag{67}$$

$$s_q^- = \sum_{nm} d_{m\downarrow}^{\dagger} d_{n\uparrow} \delta_{\uparrow\downarrow} \tag{68}$$

check operators

$$i\dot{a}_q = \omega_q a_q - J_q s_q^+ \tag{69}$$

$$i\dot{c}_{k\sigma} = \epsilon_{k\sigma,L}c_{k\sigma} + \sum_{k'} t_{k\sigma n}d_{n\sigma}$$
 (70)

$$i\dot{d}_{n\uparrow} = \epsilon_{n\uparrow}d_{n\uparrow} + \sum_{k} t_{k\uparrow n}^* c_{k\uparrow} - \sum_{q,m} J_q a_q^{\dagger} d_{m\downarrow} \delta(\epsilon_{n\uparrow} - \epsilon_{m\downarrow} - \omega_q)$$
 (71)

$$i\dot{d}_{n\downarrow} = \epsilon_{n\downarrow}d_{n\downarrow} + \sum_{k} t_{k\downarrow n}^* c_{k\downarrow} - \sum_{q,m} J_q (a_q d_{m\uparrow} - a_q^{\dagger} d_{m\uparrow}) \delta(\epsilon_{m\uparrow} - \epsilon_{n\downarrow} - \omega_q)$$
 (72)

$$-i\partial_{\tau'}G_{d,R}\left(\tau,\tau'\right) = \omega_q G_{d,R}\left(\tau,\tau'\right) - J_q G_d \tag{73}$$

or

$$G_{d,R}g_{Rq}^{-1} = -J_q G_d (74)$$

or

$$G_{d,R}(\tau,\tau') = -J_q \int G_d(\tau,\tau_1) g_{Rq}(\tau_1,\tau') d\tau_1$$
(75)

the minus before  $J_q$  originates from the minus in  $H_{sd}$ .

$$I_{s} = i \sum_{q} J_{q} \left( \left\langle s_{q}^{+} a_{q}^{\dagger} \right\rangle - \left\langle a_{q} s_{q}^{-} \right\rangle \right)$$

$$= -\sum_{q} \int \operatorname{Tr} \left[ G_{d}^{r} (\tau, \tau_{1}) \, \Sigma_{Rq}^{<} (\tau_{1}, \tau') + G_{d}^{<} (\tau, \tau_{1}) \, \Sigma_{Rq}^{a} (\tau_{1}, \tau') - h.c. \right] d\tau_{1}$$

$$(76)$$

$$\Sigma_{Rq}^{\leq} = i f_R e^{-i\omega_q(\tau - \tau')} \tag{77}$$

#### 0.3.7 Calculation of $G_d$

Definition:

$$G_{d}(\tau, \tau') = -i \left\langle T_{c} S s_{q}^{+}(\tau) s_{q}^{-}(\tau') \right\rangle$$

$$= -i \sum_{mnm'n'} \left\langle T_{c} S d_{n\uparrow}^{\dagger} d_{m\downarrow} d_{m'\downarrow}^{\dagger} d_{n'\uparrow} \right\rangle \delta\left(\epsilon_{n\uparrow} - \epsilon_{m\downarrow} - \omega_{q}\right) \delta\left(\epsilon_{n'\uparrow} - \epsilon_{m'\downarrow} - \omega_{q}\right)$$
(78)

When right lead is absent,

$$G_d(\tau, \tau') = -i \sum_{mnm'n'} G_{L,n'n\uparrow}(\tau', \tau) G_{L,mm'\downarrow}(\tau, \tau') \delta(\epsilon_{n\uparrow} - \epsilon_{m\downarrow} - \omega_q) \delta(\epsilon_{n'\uparrow} - \epsilon_{m'\downarrow} - \omega_q)$$
 (79)

where

$$G_{L,mn\sigma}(\tau,\tau') = -i\langle T_c d_{m\sigma}(\tau) d_{n\sigma}^{\dagger}(\tau') \rangle$$

$$= g_{n\sigma}(\tau,\tau') \delta_{mn}$$

$$+ \iint d\tau_1 d\tau_2 g_{m\sigma}(\tau,\tau_2) \sum_k t_{k\sigma n} t_{k\sigma m}^* g_{k\sigma}(\tau_2,\tau_1) g_{n\sigma}(\tau_1,\tau')$$

$$\cdots$$

$$= g_{n\sigma}(\tau,\tau') \delta_{mn} + \iint d\tau_1 d\tau_2 g_{m\sigma}(\tau,\tau_2) \Sigma_{L,mn\sigma}(\tau_2,\tau_1) g_{n\sigma}(\tau_1,\tau').$$
(80)

$$g_{n\sigma}(\tau, \tau') = -i \langle T_c d_n(\tau) d_{n\sigma}^{\dagger}(\tau') \rangle_0 \tag{81}$$

Self-energy of left lead

$$\Sigma_{L,mn\sigma}(\tau_2,\tau_1) = \sum_{k} t_{k\sigma n} t_{k\sigma m}^* g_{k\sigma}(\tau_2,\tau_1)$$
(82)

where

$$g_{k\sigma}(\tau_2, \tau_1) = -i \langle T_c c_{k\sigma}(\tau_2) c_{k\sigma}^{\dagger}(\tau_1) \rangle_0 \tag{83}$$

When left lead is absent,

$$G_{d}(\tau,\tau') = -i\sum_{mn} g_{n\uparrow}(\tau',\tau) g_{m\downarrow}(\tau,\tau') \delta(\varepsilon_{n\uparrow} - \varepsilon_{m\downarrow} - \omega_{q})$$

$$-\int d\tau_{1} \int d\tau_{2} \sum_{mnm'n'} g_{n\uparrow}(\tau_{1},\tau) g_{m\downarrow}(\tau,\tau_{1}) \Sigma_{R,mnm'n'}(\tau_{1},\tau_{2}) g_{n'\uparrow}(\tau',\tau_{2}) g_{m'\downarrow}(\tau_{2},\tau')$$

$$\times \delta(\varepsilon_{n\uparrow} - \varepsilon_{m\downarrow} - \omega_{q_{1}}) \delta(\varepsilon_{n'\uparrow} - \varepsilon_{m'\downarrow} - \omega_{q_{1}})$$

$$+ \cdots$$

$$= g_d(\tau, \tau') + \iint d\tau_1 d\tau_2 g_d(\tau, \tau_1) \Sigma_R(\tau_1, \tau_2) G_d(\tau_2, \tau')$$
(84)

in which,

$$g_d(\tau, \tau') = -i \sum_{mn} g_{n\uparrow}(\tau', \tau) g_{m\downarrow}(\tau, \tau') \delta(\varepsilon_{n\uparrow} - \varepsilon_{m\downarrow} - \omega_q), \tag{85}$$

the self-energy of right lead is

$$\Sigma_{R,mm'nn'}(\tau_1,\tau_2) = -i\sum_{q_1} J_{q_1}^2 g_{Rq_1}(\tau_1,\tau_2) \delta(\varepsilon_{n\uparrow} - \varepsilon_{m\downarrow} - \omega_{q_1}) \delta(\varepsilon_{n'\uparrow} - \varepsilon_{m'\downarrow} - \omega_{q_1})$$
(86)

$$g_{Rq_1}(\tau_1, \tau_2) = -i \langle T_c a_{q_1}(\tau_1) a_{q_1}^{\dagger}(\tau_2) \rangle_0$$
 (87)

Hence, when both leads are present, we have

? 
$$G_d(\tau, \tau') = -iG_{L\uparrow}(\tau', \tau) G_{L\downarrow}(\tau, \tau') - iG_{L\uparrow}(\tau_1, \tau) G_{L\downarrow}(\tau, \tau_1) \Sigma_R(\tau_1, \tau_2) G_d(\tau_2, \tau')$$
 (88)

#### 0.3.8 continuation on Eq.(88)

$$A(\tau_1, \tau') \equiv \int d\tau_2 \Sigma_R(\tau_1, \tau_2) G_d(\tau_2, \tau')$$
(89)

$$B(\tau, \tau_1) \equiv G_{L\uparrow}(\tau_1, \tau) G_{L\downarrow}(\tau, \tau_1)$$
(90)

$$C(\tau, \tau') \equiv -iG_{L\uparrow}(\tau_1, \tau) G_{L\downarrow}(\tau, \tau_1) A(\tau_1, \tau') \to$$
(91)

$$C(\tau, \tau') = -i \int d\tau_1 B(\tau, \tau_1) A(\tau_1, \tau')$$
(92)

$$D(\tau, \tau') \equiv -iG_{L\uparrow}(\tau', \tau) G_{L\downarrow}(\tau, \tau')$$
(93)

So, we have

$$G_d(\tau, \tau') = D + C \tag{94}$$

Using the analytic continuation theorem, we have

$$D^{<} = -iG_{L\uparrow}^{>}G_{L\downarrow}^{<} \tag{95}$$

$$C^{<} = -i(B^{r}A^{<} + B^{<}A^{a}) \tag{96}$$

where

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

$$\tag{97}$$

$$A^{<} = \Sigma_R^r G_d^{<} + \Sigma_R^{<} G_d^a \tag{98}$$

$$B^{<} = G_{L\uparrow}^{>} G_{L\downarrow}^{<} \tag{99}$$

$$A^a = \Sigma_R^a G_d^a \tag{100}$$

Then, the analytic continuation theorem on Eq.(88) yields

$$G_d^{<} = -iG_{L\uparrow}^{>}G_{L\downarrow}^{<} - i\left[ (G_{L\uparrow}^a G_{L\downarrow}^{<} + G_{L\uparrow}^{>}G_{L\downarrow}^r + G_{L\uparrow}^a G_{L\downarrow}^r)(\Sigma_R^r G_d^{<} + \Sigma_R^{<}G_d^a) + (G_{L\uparrow}^{>}G_{L\downarrow}^{<})(\Sigma_R^a G_d^a) \right]$$
(101)

Similarly,

$$C^{r} = -iB^{r}A^{r}$$

$$= -i(G_{L\uparrow}^{a}G_{L\downarrow}^{\langle} + G_{L\downarrow}^{\rangle}G_{L\downarrow}^{r} + G_{L\uparrow}^{a}G_{L\downarrow}^{r})(\Sigma_{R}^{r}G_{d}^{r})$$
(102)

$$D^{r} = -i(G_{L\uparrow}^{a}G_{L\downarrow}^{\langle} + G_{L\uparrow}^{\rangle}G_{L\downarrow}^{r} + G_{L\uparrow}^{a}G_{L\downarrow}^{r}), \tag{103}$$

we have

$$G_d^r = -i(G_{L\uparrow}^a G_{L\downarrow}^{<} + G_{L\uparrow}^{>} G_{L\downarrow}^r + G_{L\uparrow}^a G_{L\downarrow}^r) - i(G_{L\uparrow}^a G_{L\downarrow}^{<} + G_{L\uparrow}^{>} G_{L\downarrow}^r + G_{L\uparrow}^a G_{L\downarrow}^r)(\Sigma_R^r G_d^r). \tag{104}$$

Now we calculate  $G_d^a$ .

$$C^a = -iB^a A^a (105)$$

$$B^{a} = G_{L\uparrow}^{r} G_{L\downarrow}^{<} + G_{L\uparrow}^{>} G_{L\downarrow}^{a} + G_{L\uparrow}^{r} G_{L\downarrow}^{a} \tag{106}$$

$$D^a = -i(G_{L\uparrow}^r G_{L\downarrow}^{<} + G_{L\uparrow}^{>} G_{L\downarrow}^a + G_{L\uparrow}^r G_{L\downarrow})^a \tag{107}$$

So we have

$$G_d^a = -i(G_{L\uparrow}^r G_{L\downarrow}^{<} + G_{L\uparrow}^{>} G_{L\downarrow}^a + G_{L\uparrow}^r G_{L\downarrow}^a) - i(G_{L\uparrow}^r G_{L\downarrow}^{<} + G_{L\uparrow}^{>} G_{L\downarrow}^a + G_{L\uparrow}^r G_{L\downarrow}^a)(\Sigma_R^a G_d^a)$$
(108)

From Eq.(101) we have

$$G_{d}^{<} = -iG_{L\uparrow}^{>}G_{L\downarrow}^{<} \left(1 + \Sigma_{Rq}^{a}G_{d}^{a}\right) - i\left(G_{L\uparrow}^{a}G_{L\downarrow}^{<} + G_{L\uparrow}^{>}G_{L\downarrow}^{r} + G_{L\uparrow}^{a}G_{L\downarrow}^{r}\right)\left(\Sigma_{q}^{<}G_{d}^{a} + \Sigma_{Rq}^{r}G_{d}^{<}\right)$$

$$= \frac{-iG_{L\uparrow}^{>}G_{L\downarrow}^{<} \left(1 + \Sigma_{Rq}^{a}G_{d}^{a}\right) - i\left(G_{L\uparrow}^{a}G_{L\downarrow}^{<} + G_{L\uparrow}^{>}G_{L\downarrow}^{r} + G_{L\uparrow}^{a}G_{L\downarrow}^{r}\right)\Sigma_{R}^{<}G_{d}^{a}}{1 + i\left(G_{L\uparrow}^{a}G_{L\downarrow}^{<} + G_{L\uparrow}^{>}G_{L\downarrow}^{r} + G_{L\uparrow}^{a}G_{L\downarrow}^{r}\right)\Sigma_{R}^{r}}$$

$$(109)$$

## 0.4 Nonequilibrium Green's function technique

# Bibliography

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