

The last version is ver. ver. 2006-04-17

1 Overview

The system is made of semi-infinite left lead, a molecule, and semi-infinite right lead. L and R are in the equilibrium. The chemical potential at L is μ_L and μ_R at R. It is separated to L(semi-infinite left lead), C(molecule+lead=extended molecule) and R(semi-infinite right lead). Effects of L and R are taken into account of through the self-energy at C. It can be calculated via Green function at L or R connecting to C.

1. Green function at L or R. (surface Green function)
2. Green function at C
3. charge density at C
4. transfer matrix and conductance.

2 tight binding Hamiltonian

eigenfunction $|\psi_\nu\rangle$ is made of LCAO at (site,orbital) i , $|\phi_i\rangle$.

$$H = T + V_{\text{external}} + V_{\text{ion}} + V_{\text{Coulomb}} + V_{\text{exchange-correlation}} \quad (1)$$

$$H|\psi_\nu\rangle = E_\nu|\psi_\nu\rangle \quad (2)$$

$$|\psi_\nu\rangle = \sum_i c_{\nu i}|\phi_i\rangle \quad (3)$$

$$H_{ij} = \langle\phi_i|H|\phi_j\rangle \quad (4)$$

$$S_{ij} = \langle\phi_i|\phi_j\rangle \quad (5)$$

Not necessary that ϕ_i is orthogonal. V_{external} comes from, e.g., bias voltage. E_ν, S are calculated by solving

$$H = ES \quad (6)$$

3 surface Green function, orthogonal basis

3.1 normal

Green function

$$(\omega - H)G = I \quad (7)$$

consider periodic layers with an edge. There exist transfer integrals only between neighboring layers. The layer 0 has the edge.

$$H = \begin{bmatrix} H_{00} & H_{01} & 0 & 0 & 0 \\ H_{10} & H_{11} & H_{12} & 0 & 0 \\ 0 & H_{21} & H_{22} & H_{23} & 0 \\ 0 & 0 & H_{32} & H_{33} & \ddots \\ 0 & 0 & 0 & \ddots & \ddots \end{bmatrix} \quad (8)$$

By definition, $H_{01} = H_{i,i+1} = H_{i+1,i}^\dagger$, $H_{00} = H_{ii} = H_{i+1,i+1}$.

Green function

$$G = \begin{bmatrix} G_{00} & G_{01} & G_{02} & G_{13} & \ddots \\ G_{10} & G_{11} & G_{12} & & \\ G_{20} & G_{21} & G_{22} & & \\ G_{30} & & & G_{33} & \\ \vdots & & & & \ddots \end{bmatrix} \quad (9)$$

Use G_{i0} column,

$$(\omega - H_{00})G_{00} - H_{01}G_{10} = I \quad (10)$$

$$-H_{10}G_{00} + (\omega - H_{11})G_{10} - H_{12}G_{20} = 0 \quad (11)$$

$$-H_{21}G_{10} + (\omega - H_{22})G_{20} - H_{23}G_{30} = 0 \quad (12)$$

$$\vdots \quad (13)$$

eq.(10) to eq.(12) is generalized as

$$(\omega - H_{nn})G_{n0} = H_{n,n-1}G_{n-1,0} + H_{n,n+1}G_{n+1,0} \quad (14)$$

eq.(10) and eq.(14) describes relation between the neighboring layer. rewrite eq.(10) and eq.(14) as

$$(\omega - \epsilon_0^s)G_{00} = I + \alpha_0 G_{10} \quad (15)$$

$$(\omega - \epsilon_0)G_{n0} = \beta_0 G_{n-1,0} + \alpha_0 G_{n+1,0} \quad (16)$$

The relationship between the second neighboring layer corresponding to eq.(15) is

$$\begin{aligned} (\omega - \epsilon_0^s)G_{00} &= I + \alpha_0(\omega - \epsilon_0)^{-1}(\beta_0 G_{0,0} + \alpha_0 G_{2,0}) \\ \{\omega - (\epsilon_0^s + \alpha_0(\omega - \epsilon_0)^{-1}\beta_0)\}G_{00} &= I + \alpha_0(\omega - \epsilon_0)^{-1}\alpha_0 G_{2,0} \\ (\omega - \epsilon_1^s)G_{00} &= I + \alpha_1 G_{20} \end{aligned} \quad (17)$$

The relationship between the second neighboring layer corresponding to eq.(16) is

$$\begin{aligned} (\omega - \epsilon_0)G_{n0} &= \beta_0(\omega - \epsilon_0)^{-1}(\beta_0 G_{n-2,0} + \alpha_0 G_{n,0}) \\ &\quad + \alpha_0(\omega - \epsilon_0)^{-1}(\beta_0 G_{n,0} + \alpha_0 G_{n+2,0}) \\ \{\omega - (\epsilon_0 + \beta_0(\omega - \epsilon_0)^{-1}\alpha_0 + \alpha_0(\omega - \epsilon_0)^{-1}\beta_0)\}G_{n0} &= \beta_0(\omega - \epsilon_0)^{-1}\beta_0 G_{n-2,0} + \alpha_0(\omega - \epsilon_0)^{-1}\alpha_0 G_{n+2,0} \\ (\omega - \epsilon_1)G_{n0} &= \beta_1 G_{n-2,0} + \alpha_1 G_{n+2,0} \end{aligned} \quad (18)$$

$$\quad (19)$$

From eq.(15), eq.(16), eq.(17), eq.(19), the relation between 2^i th neighboring layer is

$$(\omega - \epsilon_i^s)G_{00} = I + \alpha_i G_{2^i,0} \quad (20)$$

$$(\omega - \epsilon_i)G_{n0} = \beta_i G_{n-2^i,0} + \alpha_i G_{n+2^i,0} \quad (21)$$

$\epsilon_i^s, \epsilon_i, \alpha_i, \beta_i$ can be evaluated iteratively

$$\epsilon_{i+1}^s = \epsilon_i^s + \alpha_i(\omega - \epsilon_i)^{-1}\beta_i \quad (22)$$

$$\epsilon_{i+1} = \epsilon_i + \beta_i(\omega - \epsilon_i)^{-1}\alpha_i + \alpha_i(\omega - \epsilon_i)^{-1}\beta_i \quad (23)$$

$$\alpha_{i+1} = \alpha_i(\omega - \epsilon_i)^{-1}\alpha_i \quad (24)$$

$$\beta_{i+1} = \beta_i(\omega - \epsilon_i)^{-1}\beta_i \quad (25)$$

The initial values are

$$\epsilon_0^s = H_{00} \quad (26)$$

$$\epsilon_0 = H_{00} \quad (27)$$

$$\alpha_0 = H_{01} \quad (28)$$

$$\beta_0 = H_{10} \quad (29)$$

if $|\alpha_i| \rightarrow 0$ for $i \rightarrow \infty$,¹ and also use eq.(22),

$$G_{00} = (\omega - \epsilon_i^s)^{-1}|_{i \rightarrow \infty} \quad (30)$$

3.2 use transfer matrix

Rewrite eq.(16)

$$G_{n0} = t_0 G_{n-1,0} + \tilde{t}_0 G_{n+1,0} \quad (31)$$

$$t_0 = (\omega - H_{00})^{-1} H_{01}^\dagger \quad (32)$$

$$\tilde{t}_0 = (\omega - H_{00})^{-1} H_{01} \quad (33)$$

Then the relation between the next nearest neighbor is

$$G_{n0} = t_0(t_0 G_{n-2,0} + \tilde{t}_0 G_{n,0}) + \tilde{t}_0(t_0 G_{n,0} + \tilde{t}_0 G_{n+2,0}) \quad (34)$$

$$G_{n0} = (I - t_0 \tilde{t}_0 - \tilde{t}_0 t_0)^{-1} (t_0 t_0 G_{n-2,0} + \tilde{t}_0 \tilde{t}_0 G_{n+2,0}) \quad (35)$$

rewrite it

$$G_{n0} = t_1 G_{n-2,0} + \tilde{t}_1 G_{n+2,0} \quad (36)$$

$$t_1 = (I - t_0 \tilde{t}_0 - \tilde{t}_0 t_0)^{-1} (t_0)^2 \quad (37)$$

$$\tilde{t}_1 = (I - t_0 \tilde{t}_0 - \tilde{t}_0 t_0)^{-1} (\tilde{t}_0)^2 \quad (38)$$

generally

$$G_{n0} = t_i G_{n-2^i,0} + \tilde{t}_i G_{n+2^i,0} \quad (39)$$

$$t_i = (I - t_{i-1} \tilde{t}_{i-1} - \tilde{t}_{i-1} t_{i-1})^{-1} (t_{i-1})^2 \quad (40)$$

$$\tilde{t}_i = (I - t_{i-1} \tilde{t}_{i-1} - \tilde{t}_{i-1} t_{i-1})^{-1} (\tilde{t}_{i-1})^2 \quad (41)$$

at eq.(39), set $n = 2^i$

$$G_{2^i,0} = t_i G_{0,0} + \tilde{t}_i G_{2^{i+1},0} \quad (42)$$

use eq.(42) iteratively

$$G_{10} = t_0 G_{0,0} + \tilde{t}_0 G_{2,0} \quad (43)$$

$$(G_{2,0} = t_1 G_{0,0} + \tilde{t}_1 G_{4,0}) \quad (44)$$

$$= (t_0 + \tilde{t}_0 t_1) G_{0,0} + \tilde{t}_0 \tilde{t}_1 G_{4,0} \quad (45)$$

$$(G_{4,0} = t_2 G_{0,0} + \tilde{t}_2 G_{8,0}) \quad (46)$$

$$= (t_0 + \tilde{t}_0 t_1 + \tilde{t}_0 \tilde{t}_1 t_2) G_{0,0} + \tilde{t}_0 \tilde{t}_1 \tilde{t}_2 G_{8,0} \quad (47)$$

$$= \dots = (t_0 + \tilde{t}_0 t_1 + \tilde{t}_0 \tilde{t}_1 t_2 + \dots + \tilde{t}_0 \tilde{t}_1 \dots \tilde{t}_{i-1} t_i) G_{0,0} + \tilde{t}_0 \tilde{t}_1 \dots \tilde{t}_{i-1} \tilde{t}_i G_{2^{i+1},0} \quad (48)$$

$$= T_i G_{0,0} + \tilde{t}_0 \tilde{t}_1 \dots \tilde{t}_{i-1} \tilde{t}_i G_{2^{i+1},0} \quad (49)$$

$$T_i = t_0 + \tilde{t}_0 t_1 + \tilde{t}_0 \tilde{t}_1 t_2 + \dots + \tilde{t}_0 \tilde{t}_1 \dots \tilde{t}_{i-1} t_i \quad (50)$$

If $|\tilde{t}_0 \tilde{t}_1 \dots \tilde{t}_{i-1} \dots| \rightarrow 0$ for $i \rightarrow \infty$,²

$$G_{10} = T G_{00} \quad (51)$$

where $T = T_i|_{i \rightarrow \infty}$
from eq.(15) using T

$$(\omega - H_{00}) G_{00} - H_{01} G_{10} = I \quad (52)$$

$$G_{00} = (\omega - H_{00} - H_{01} T)^{-1} \quad (53)$$

¹" $G_{2^i,0}$ will be 0 when $i \rightarrow \infty$ " is wrong.

²" $G_{2^i,0}$ will be 0 when $i \rightarrow \infty$ " is wrong.

3.3 $G_{n0}|_{n \rightarrow \infty} \rightarrow 0$?

This is not true. Consider the case where there exists a single site in the unit cel and $H_{00} = 0$ (energy level) and $H_{10} = t$ (transfer integral to the nn site).

$$G_{2n,0}|_{n \rightarrow \infty}(\omega) \sim t^{2n-1}/\text{Det}(\omega I - H) \quad (54)$$

If $\omega = 0$, or ω is equal to the energy level,

$$\text{Det}(\omega I - H) = (-1)t^{2n} \quad (55)$$

Then,

$$G_{2n,0}(\omega = 0)|_{n \rightarrow \infty} \sim 1/t \quad (56)$$

4 Green function of the extended molecule, orthogonal basis

4.1 block matrix

$$(\omega - H)G = I$$

consider L,C and R region and rewrite it

$$(w - H) = \begin{bmatrix} \omega - H_L & -H_{LC} & 0 \\ -H_{CL} & \omega - H_C & -H_{CR} \\ 0 & -H_{RC} & \omega - H_R \end{bmatrix} \quad (57)$$

G_C , the Green function at the C region, can be calculates as³

$$G_C = \{\omega - H_C - H_{CR}(\omega - H_R)^{-1}H_{RC} - H_{CL}(\omega - H_L)^{-1}H_{LC}\}^{-1} \quad (58)$$

$$= \{\omega - H_C - \Sigma_R - \Sigma_L\}^{-1} \quad (59)$$

$$\Sigma_R = H_{CR}(\omega - H_R)^{-1}H_{RC} = H_{CR}G_R H_{RC} \quad (60)$$

$$\Sigma_L = H_{CL}(\omega - H_L)^{-1}H_{LC} = H_{CL}G_L H_{LC} \quad (61)$$

G_R and G_L corresponds to the surface Green function, G_{00} , in the previous section.

Note that $G_C(\omega)$ is calculated for $G_C^R(\omega) = G_C(\omega + i\delta)$ and $G_C^A(\omega) = G_C(\omega - i\delta)$.

define for the later convenience

$$\Gamma_R = i(\Sigma_R^R - \Sigma_R^A) \quad (62)$$

$$\Gamma_L = i(\Sigma_L^R - \Sigma_L^A) \quad (63)$$

$$(64)$$

In the equilibrium condition,⁴

$$G^< = iAf(E - \mu) \quad (65)$$

$$A = i(G^R - G^A) \quad (66)$$

$$G^< = -(G^R - G^A)f(E - \mu) \quad (67)$$

while

$$G^< = G^R \Sigma^< G^A \quad (68)$$

³for $A = \begin{bmatrix} a_{11} & a_{12} & 0 \\ a_{21} & a_{22} & a_{23} \\ 0 & a_{32} & a_{33} \end{bmatrix}$, $A_{22}^{-1} = \frac{a_{11}a_{33}}{a_{11}a_{22}a_{33} - a_{11}a_{23}a_{32} - a_{33}a_{12}a_{21}}$

⁴corrected May 12, 2005

therefore

$$\Sigma^< = -G^{R-1}(G^R - G^A)f(E - \mu)G^{A-1} \quad (69)$$

$$= -(G^{A-1} - G^{R-1})f(E - \mu) \quad (70)$$

$$= -(\Sigma^R - \Sigma^A)f(E - \mu) \quad (71)$$

How are Σ_R and Σ_L ? They are defined in non-equilibrium region, C. but near the region L or R, they approximately satisfy equilibrium condition.

$$\Sigma_R^< = -(\Sigma_R^R - \Sigma_R^A)f(E - \mu_R) \quad (72)$$

$$\Sigma_L^< = -(\Sigma_L^R - \Sigma_L^A)f(E - \mu_L) \quad (73)$$

5 total charge

5.1 in the equilibrium

5.1.1 total charge from the retarded Green function

total charge, n_{tot} , is calculated from the retarded Green function

$$A_{ij}(\omega) = -\frac{1}{\pi}\text{Im}G_{ij}^R(\omega) \quad (74)$$

$$\rho_{ij} = \int^{\mu} d\omega A_{ij}(\omega) \quad (75)$$

$$= -\frac{1}{\pi}\text{Im} \int^{\mu} d\omega G_{ij}^R(\omega) \quad (76)$$

$$n_{tot} = \text{Tr}[\rho] \quad (77)$$

where $G^R(\omega) = G(\omega + i\delta)$

5.1.2 total charge from contour integration

usually eq.(76) is unstable. employ contour integration

$$\rho_{ij} = \frac{1}{2\pi i} \int_C dz G_{ij}(z) \quad (78)$$

$$= \frac{1}{2\pi i} \int_{C_1} dz G_{ij}(z) + \frac{1}{2\pi i} \int_{C_2} dz G_{ij}(z) \quad (79)$$

$$= \frac{1}{\pi} \text{Im} \int_{C_1} dz G_{ij}(z) \quad (80)$$

where the path $C = (\mu, 0) \rightarrow (\mu, i\Gamma) \rightarrow (E_{min}, i\Gamma) \rightarrow (E_{min}, -i\Gamma) \rightarrow (\mu, -i\Gamma) \rightarrow (\mu, 0)$, and C_1 is the lower half of C and C_2 is the upper half of C. i.e. $C_1 = (E_{min}, 0) \rightarrow (E_{min}, -i\Gamma) \rightarrow (\mu, -i\Gamma) \rightarrow (\mu, 0)$,

E_{min} is smaller than the minimum of the eigenvalues.

5.1.3 total charge from contour integration 2

TRANSIESTA uses a different approach. eq.(75) can be written as

$$\rho_{ij} = \int_{-\infty}^{\infty} d\omega A_{ij}(\omega)f(\omega - \mu) \quad (81)$$

$$= -\frac{1}{\pi} \text{Im} \int_{-\infty}^{\infty} d\omega G_{ij}^R(\omega)f(\omega - \mu) \quad (82)$$

where $f(\omega - \mu)$ is the Fermi distribution function. using the thermal Green function and the pole of $f(\omega)$ is at $i\omega_n$,

$$\left(\int_{L_1} + \int_{L_2} + \int_{L_3} \right) d\omega G^R(\omega) f(\omega - \mu) = -2\pi i \frac{1}{\beta} \sum_{i\omega_n}^{iQ} G(i\omega_n) \quad (83)$$

where the path L_1 is $(E_{min}, 0) \rightarrow (\infty, 0)$, L_2 is $(\infty, iQ) \rightarrow (\mu, iQ)$ and L_3 is $(\mu, iQ) \rightarrow (E_{min}, 0)$. E_{min} is smaller than the minimum of the eigenvalues. Q is a small value enough to stabilize the integration. Then

$$\rho_{ij} = -\frac{1}{\pi} \text{Im} \left[\int_{L_2+L_3} d\omega G^R(\omega) f(\omega - \mu) - 2\pi i \frac{1}{\beta} \sum_{i\omega_n}^{iQ} G(i\omega_n) \right] \quad (84)$$

practical upper limit to calculate $\int_{L_2} d\omega$ is $\sim \mu + 10T$ due to the presence of $f(\omega - \mu)$

Note that G^R has no pole in the upper half plane of ω

5.1.4 total charge using modified matsubara summaiton

$$e^Z \simeq (1 + Z/n)^n \quad (85)$$

then

$$f(Z) = \frac{1}{1 + e^{\beta(Z-\mu)}} \simeq \bar{f}(Z) = \frac{1}{1 + \left(1 + \frac{\beta(Z-\mu)}{2M}\right)^{2M}} \quad (86)$$

$f(Z) = \bar{f}(Z)$ when $M \rightarrow \infty$
 $\bar{f}(Z)$ has poles at

$$E_p = \mu + \frac{2M}{\beta}(z_p - 1) \quad (87)$$

$$z_p = \exp\left(\frac{i\pi(2p+1)}{2M}\right) \quad (88)$$

total charge is

$$\rho \simeq \int_{-\infty}^{\infty} d\omega A(\omega) \bar{f}(\omega) \quad (89)$$

From the counter integration of the upper-half plane,

$$\int_{-\infty}^{\infty} d\omega A(\omega) \bar{f}(\omega) = 2\pi i \sum_{p=0}^{M-1} A(E_p) R_p \quad (90)$$

where R_p is residue and equals $-z_p/\beta$.

5.2 in the non-equilibrium

$$G_C^<(t) = i \langle c_i^+ c_j(t) \rangle$$

One must calculate

$$\rho_{ij} = \langle c_i^+ c_j(0) \rangle \quad (91)$$

$$= \frac{1}{i} G_C^<(0) \quad (92)$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega G_C^<(\omega) \quad (93)$$

This can be evaluated only approximately.

Because $G^{A^{-1}} - G^{R^{-1}} = \Sigma^R - \Sigma^A = -i\Gamma$,

$$2\pi A = i(G^R - G^A) = G^R \Gamma G^A = G^R (\Gamma_R + \Gamma_L) G^A \quad (94)$$

A is the spectrum function.

At region C ,

$$2\pi A = G^R \Gamma G^A = G^R (\Gamma_R + \Gamma_L) G^A \quad (95)$$

where $\Gamma = \Gamma_R + \Gamma_L$ because $\Sigma = \Sigma_R + \Sigma_L$.

Assume that the region of C near the region L and R is close to the equilibrium. If not, the self-energy defined in the region C can not be evaluated.

$$G_C^< = G_C^R \Sigma^< G_C^A \quad (96)$$

$$\simeq G_C^R i(\Gamma_L f(\omega - \mu_L) + \Gamma_R f(\omega - \mu_R)) G_C^A \quad (97)$$

$$= -G_C^R ((\Sigma_L^R - \Sigma_L^A) f(\omega - \mu_L) + (\Sigma_R^R - \Sigma_R^A) f(\omega - \mu_R)) G_C^A \quad (98)$$

Note that the left side of eq.(98) is not analytical.

If $\omega < \min(\mu_L, \mu_R) - 10T$, $f(\omega - \mu) = 1$. then

$$G^< = 2\pi i A \quad (99)$$

then eq.(93) is

$$\rho_{ij} = \int_{-\infty}^{E_1} d\omega A_{ij}(\omega) + \int_{E_1}^{\infty} \frac{d\omega}{2\pi i} G_{ij}^<(\omega) \quad (100)$$

The first term can be calculated in the same manner as the case of the equilibrium condition. For $\omega \ll \mu$, the electronic structure of the system will be close to the equilibrium. E_1 ($< \min(\mu_L, \mu_R) - 10T$) is the energy below which the electronic structure is close enough to the equilibrium state. Note $G^<(\omega)$ goes 0 for $\omega > \max(\mu_L, \mu_R) + 10T$. the upper limit of the second term can be not an infinite.

5.3 in the non-equilibrium, TRANSIESTA's approach

From eqs.(93) and (98),

$$\rho_{ij} = \int_{-\infty}^{\infty} d\omega \rho_{ij}^L(\omega) f(\omega - \mu_L) + \int_{-\infty}^{\infty} d\omega \rho_{ij}^R(\omega) f(\omega - \mu_R) \quad (101)$$

$$= \int_{-\infty}^{\infty} d\omega (\rho_{ij}^L(\omega) + \rho_{ij}^R(\omega)) f(\omega - \mu_R) \quad (102)$$

$$+ \int_{-\infty}^{\infty} d\omega \rho_{ij}^L(\omega) (f(\omega - \mu_L) - f(\omega - \mu_R)) \quad (103)$$

Assuming $\mu_L > \mu_R$, we can replace $\rho_{ij}^L(\omega) + \rho_{ij}^R(\omega)$ with $A(\omega)$ for $\omega \leq \mu_R$.

$$\rho_{ij} = \int_{-\infty}^{\infty} d\omega A(\omega) f(\omega - \mu_R) \quad (104)$$

$$+ \int_{-\infty}^{\infty} d\omega \rho_{ij}^L(\omega) (f(\omega - \mu_L) - f(\omega - \mu_R)) \quad (105)$$

We evaluate the first term in eq.(84). $\rho^L(\omega)$ in the second term is not analytical.

6 current

References in this section is ref.[1, 6, 7], which are rarely cited. I wonder why. Transmission is evaluated as

$$T(\omega) = \text{Tr} [\Gamma_L(\omega)G^R(\omega)\Gamma_R(\omega)G^A(\omega)] \quad (106)$$

current is

$$I = \frac{e}{\hbar} \int d\omega T(\omega)(f(\omega - \mu_L) - f(\omega - \mu_R)) \quad (107)$$

6.1 derivation 1. time-dependent

$$H = \sum \epsilon_\alpha^0 c_\alpha^\dagger c_\alpha + \sum \epsilon_i^0 d_i^\dagger d_i + H_{int}(\{d_i^\dagger\}, \{d_i\}) + \sum (t_{i\alpha} d_i^\dagger c_\alpha + \text{h.c.}) \quad (108)$$

current from L region is

$$J_L = -(-e)\langle \dot{N}_L \rangle = ie\langle [H, N_L] \rangle \quad (109)$$

$$[H, N_L] = [H, \sum d_k^\dagger d_k] \quad (110)$$

$$= [t_{i\alpha} d_i^\dagger c_\alpha + t_{\alpha i} c_\alpha^\dagger d_i, \sum d_k^\dagger d_k] \quad (111)$$

$$= -t_{i\alpha} d_i^\dagger c_\alpha + t_{\alpha i} c_\alpha^\dagger d_i \quad (112)$$

$$J_L = ie \sum (-t_{i\alpha} \langle d_i^\dagger c_\alpha \rangle + t_{\alpha i} \langle c_\alpha^\dagger d_i \rangle) \quad (113)$$

interesting that the prefactor of the current is imaginary!

Define Keldysh Green functions

$$G_{j\alpha}^<(t, t') = i \langle c_\alpha^\dagger(t') d_j(t) \rangle \quad (114)$$

$$G_{ji}^<(t, t') = i \langle d_i^\dagger(t') d_j(t) \rangle \quad (115)$$

$$g_\alpha^<(t, t') = i \langle c_\alpha^\dagger(t') c_\alpha(t) \rangle \quad (116)$$

Dyson equation, $\leftarrow\leftarrow\leftarrow + \leftarrow \Sigma \leftarrow\leftarrow$, reads

$$\begin{pmatrix} i \leftarrow i & i \leftarrow \alpha \\ \alpha \leftarrow i & \alpha \leftarrow \alpha \end{pmatrix} = \begin{pmatrix} i \leftarrow i & 0 \\ 0 & \alpha \leftarrow \alpha \end{pmatrix} \quad (117)$$

$$+ \begin{pmatrix} i \leftarrow i & 0 \\ 0 & \alpha \leftarrow \alpha \end{pmatrix} \begin{pmatrix} \Sigma & t \\ t^\dagger & 0 \end{pmatrix} \begin{pmatrix} i \leftarrow i & i \leftarrow \alpha \\ \alpha \leftarrow i & \alpha \leftarrow \alpha \end{pmatrix} \quad (118)$$

\leftarrow means non-interacting Green function and is diagonal. $\leftarrow\leftarrow$ means interacting Green function which includes self-energies. i is indexes in the region C and α is in the region L, e.g.,

$$i \leftarrow i = \begin{pmatrix} 1 \leftarrow 1 & 0 & 0 \\ 0 & 2 \leftarrow 2 & 0 \\ 0 & 0 & 3 \leftarrow 3 \\ & & & \ddots \end{pmatrix} \quad (119)$$

and so on.

The second term reads

$$\begin{pmatrix} (i \leftarrow i, \Sigma, \alpha \leftarrow i) + (i \leftarrow i, t_{i\alpha}, \alpha \leftarrow i) & (i \leftarrow i, \S, i \leftarrow \alpha) + (i \leftarrow i, t_{i\alpha}, \alpha \leftarrow \alpha) \\ \alpha \leftarrow \alpha, t_{\alpha i}, i \leftarrow i & \alpha \leftarrow \alpha, t_{\alpha i}, i \leftarrow \alpha \end{pmatrix} \quad (120)$$

The (2,1) component of eq.(118) gives

$$(\alpha \leftarrow i) = (\alpha \leftarrow \alpha, t_{\alpha i}, i \leftarrow i) \quad (121)$$

Thus for equilibrium Green functions,

$$G_{i\alpha}(t, t') = \int dt_1 \sum_j G_{ij}(t, t_1) t_{j\alpha}(t_1) g_\alpha(t_1, t) \quad (122)$$

For non equilibrium Green functions,

$$G_{i\alpha}^<(t, t') = \int dt_1 \left\{ \sum_j G_{ij}^R(t, t_1) t_{j\alpha}(t_1) g_\alpha^<(t_1, t) + \sum_j G_{ij}^<(t, t_1) t_{j\alpha}(t_1) g_\alpha^A(t_1, t) \right\} \quad (123)$$

time dependence of $\epsilon_\alpha(t)$

$$\epsilon_\alpha(t) = \epsilon_\alpha^0 + \Delta_\alpha(t) \quad (124)$$

In the stochastic approximation,

$$g_\alpha^<(t, t') = if(\epsilon_\alpha^0) \exp(-i \int_{t'}^t dt_2 \epsilon_\alpha(t_2)) \quad (125)$$

$$g_\alpha^A(t, t') = i\theta(t' - t) \exp(-i \int_{t'}^t dt_2 \epsilon_\alpha(t_2)) \quad (126)$$

return to eq.(113), ⁵

$$J_L(t) = e \sum [t_{\alpha i} G_{i\alpha}^<(t, t) + \text{h.c.}] \quad (127)$$

$$= 2e \text{Re} \sum_{\alpha i} t_{\alpha i} G_{i\alpha}^<(t, t) = 2e \text{Re tr} [tG^<] \quad (128)$$

See also the Appendix.

Use eq.(123), eq.(125) and eq.(126)

$$\sum_{\alpha i} t_{\alpha i} G_{i\alpha}^<(t, t) = \sum_{\alpha i} t_{\alpha i} \sum_j \int dt_1 [G_{ij}^R(t, t_1) t_{j\alpha}(t_1) g_\alpha^<(t_1, t) + G_{ij}^<(t, t_1) t_{j\alpha}(t_1) g_\alpha^A(t_1, t)] \quad (129)$$

$$= i \sum_{\alpha i j} \int dt_1 t_{\alpha i}(t_1) t_{j\alpha}(t_1) [G_{ij}^R(t, t_1) f(\epsilon_\alpha^0) + G_{ij}^<(t, t_1) \theta(t - t_1)] \times \exp\left(-i \int_t^{t_1} dt_2 \epsilon_\alpha(t_2)\right) \quad (130)$$

insert $\int d\epsilon \delta(\epsilon - \epsilon_\alpha^0)$

$$\sum_{\alpha i} t_{\alpha i} G_{i\alpha}^<(t, t) = i \sum_{\alpha i j} \int dt_1 \int d\epsilon \sum_\alpha \delta(\epsilon - \epsilon_\alpha^0) t_{\alpha i}(t) t_{j\alpha}(t) \exp(-i\epsilon_\alpha^0(t_1 - t)) \times \exp\left(-i \int_{t_1}^t dt_2 \Delta_\alpha(t_2)\right) [G_{ij}^R(t, t_1) f(\epsilon_\alpha^0) + G_{ij}^<(t, t_1) \theta(t - t_1)] \quad (131)$$

Define

$$\Gamma_{ji}(\epsilon, t_1, t) = 2\pi \sum_\alpha \delta(\epsilon - \epsilon_\alpha^0) t_{\alpha i}(t) t_{j\alpha}(t_1) \exp\left(-i \int_t^{t_1} dt_2 \Delta_\alpha(t_2)\right) \quad (132)$$

Then

$$\sum_{\alpha i} t_{\alpha i} G_{i\alpha}^<(t, t) = i \sum_{ij} \int dt_1 \int \frac{d\epsilon}{2\pi} e^{i\epsilon(t-t_1)} \Gamma_{ji}(\epsilon, t_1, t) [G_{ij}^R(t, t_1) f(\epsilon_\alpha^0) + G_{ij}^<(t, t_1) \theta(t - t_1)] \quad (133)$$

⁵The result, real or imaginary part, depends on the definition. Usually it is written as $2e \text{Im tr}[tG^<]$, which may be more comfortable.

Taking into account of $G_{ij}^R(t, t_1) = -i\theta(t - t_1)\langle d_j(t_1), d_i(t)^\dagger \rangle$, upper limit of $\int dt_1$ is t .

$$\sum_{\alpha i} t_{\alpha i} G_{i\alpha}^<(t, t) = i \sum_{ij} \int_{-\infty}^t dt_1 \int \frac{d\epsilon}{2\pi} e^{i\epsilon(t-t_1)} \Gamma_{ji}(\epsilon, t_1, t) [G_{ij}^R(t, t_1) f(\epsilon) + G_{ij}^<(t, t_1)] \quad (134)$$

Therefore

$$J_L(t) = 2e \int_{-\infty}^t dt_1 \int \frac{d\epsilon}{2\pi} \text{Im Tr} \left[e^{i\epsilon(t-t_1)} \Gamma(e, t_1, t) (G^R(t, t_1) f(\epsilon) + G^<(t, t_1)) \right] \quad (135)$$

6.2 derivation 2. time-independent

from eq.(129)

$$\begin{aligned} \sum_{\alpha i} t_{\alpha i} G_{i\alpha}^<(t, t) &= \sum_{\alpha i} t_{\alpha i} \sum_j \int dt_1 \left[\int \frac{d\omega_1}{2\pi} G_{ij}^R(\omega_1) e^{-i\omega_1(t-t_1)} t_{j\alpha} \int \frac{d\omega_2}{2\pi} g_{\alpha}^<(\omega_2) e^{-i\omega_2(t-t_1)} \right. \\ &\quad \left. + \int \frac{d\omega_1}{2\pi} G_{ij}^<(\omega_1) e^{-i\omega_1(t-t_1)} t_{j\alpha} \int \frac{d\omega_2}{2\pi} g_{\alpha}^A(\omega_2) e^{-i\omega_2(t-t_1)} \right] \end{aligned} \quad (136)$$

$$= \sum_{\alpha ij} t_{\alpha i} t_{j\alpha} \int \frac{d\omega_1}{2\pi} [G_{ij}^R(\omega_1) g_{\alpha}^<(\omega_1) + G_{ij}^<(\omega_1) g_{\alpha}^A(\omega_1)] \quad (137)$$

time independent $\rightarrow \epsilon_{\alpha} = \epsilon_{\alpha}^0$ (eigenvalue of the isolated L region)

Green functions become

$$g_{\alpha}^<(\omega) = i \int dt e^{i\omega t} f(\epsilon_{\alpha}) e^{-i\epsilon_{\alpha} t} = 2\pi i \delta(\omega - \epsilon_{\alpha}) \quad (138)$$

$$g_{\alpha}^R(\omega) = -i \int dt e^{i\omega t - \delta t} \theta(t) e^{-i\epsilon_{\alpha} t} = \frac{1}{\omega - \epsilon_{\alpha} + i\delta} \quad (139)$$

$$g_{\alpha}^A(\omega) = i \int dt e^{i\omega t - \delta t} \theta(-t) e^{-i\epsilon_{\alpha} t} = \frac{1}{\omega - \epsilon_{\alpha} - i\delta} \quad (140)$$

J_L becomes

$$J_L = 2e \text{Re} \sum_{\alpha ij} t_{\alpha n} t_{m\alpha} \int \frac{d\omega_1}{2\pi} \left[G_{ij}^R(\omega_1) 2\pi i \delta(\omega - \epsilon_{\alpha}) f(\omega_1) + G_{ij}^<(\omega_1) \frac{1}{\omega - \epsilon_{\alpha} - i\delta} \right] \quad (141)$$

$$\begin{aligned} &= 2e \text{Im} \int d\omega_1 \left(\sum_{\alpha} t_{\alpha n} t_{m\alpha} \delta(\omega - \epsilon_{\alpha}) \right) \left\{ G_{ij}^R(\omega_1) f(\omega_1) + \frac{1}{2} G_{ij}^<(\omega_1) \right\} \\ &\quad + 2e \text{Re} \int \frac{d\omega_1}{2\pi} \left(\sum_{\alpha} t_{\alpha n} t_{m\alpha} \text{P} \frac{1}{\omega - \epsilon_{\alpha}} \right) G_{ij}^<(\omega_1) \end{aligned} \quad (142)$$

Here define

$$\Gamma_{ij}(\omega) = 2\pi \sum_{\alpha} t_{\alpha i} t_{j\alpha} \delta(\omega - \epsilon_{\alpha}) \quad (143)$$

$$= i \sum_{\alpha} t_{\alpha i} t_{j\alpha} \left(\frac{1}{\omega - \epsilon_{\alpha} + i\delta} - \frac{1}{\omega - \epsilon_{\alpha} - i\delta} \right) \quad (144)$$

$$= i \sum_{\alpha} t_{\alpha i} t_{j\alpha} (g_{\alpha}^R(\omega) - g_{\alpha}^A(\omega)) \quad (145)$$

$$= i(\Sigma^R(\omega) - \Sigma^A(\omega)) \quad (146)$$

Use $\text{Im}G^R = \frac{1}{2i}(G^R - G^A)$,

$$\begin{aligned} J_L &= -ei \int \frac{d\omega}{2\pi} \sum_{ij} \Gamma_{ij}(\omega) \{ (G_{ij}^R - G_{ij}^A) f(\omega) + G_{ij}^< \} \\ &\quad + 2e\text{Re} \int \frac{d\omega}{2\pi} \sum_{ij} \left(\sum_{\alpha} t_{\alpha i} t_{j\alpha} \frac{P}{\omega - \epsilon_{\alpha}} \right) G_{ij}^< \end{aligned} \quad (147)$$

If region described by $\{d_i\}, \{d_i^{\dagger}\}$ is non-interacting, then $G_{ij}^<$ is pure imaginary.

$$J_L = -ei \int \frac{d\omega}{2\pi} \text{Tr} [\Gamma(\omega) \{ (G^R - G^A) f(\omega) + G^< \}] \quad (148)$$

Note that $\Gamma(\omega)$ and $f(\omega)$ are defined for the equilibrium L region.

Let's connect L-C-R. Use equations,

$$G^< = G^R \Sigma^< G^A \quad (149)$$

$$\Sigma^< = i f_L(\omega) \Gamma_L + i f_R(\omega) \Gamma_R \quad (150)$$

$$\Gamma_L + \Gamma_R = i(G^A{}^{-1} - G^R{}^{-1}) \quad (151)$$

$$G^R - G^A = -iG^R(\Gamma_L + \Gamma_R)G^A \quad (152)$$

$f_L(\omega)$ means $f(\omega - \mu_L)$ where μ_L is the chemical potential in the L region. $f_R(\omega)$ means $f(\omega - \mu_R)$. Note again that eq.(150) is evaluated assuming the system is in the equilibrium.

$$J = J_L = -J_R \quad (153)$$

$$= (J_L - J_R)/2 \quad (154)$$

$$= \frac{e}{2i} \int \frac{d\omega}{2\pi} \text{Tr} [\Gamma_L(G^R - G^A) f_L + \Gamma_L G^< - \Gamma_R(G^R - G^A) f_R - \Gamma_R G^<] \quad (155)$$

$$= \frac{e}{2i} \int \frac{d\omega}{2\pi} \text{Tr} [(\Gamma_L f_L - \Gamma_R f_R)(-i)G^R(\Gamma_L + \Gamma_R)G^A + i(\Gamma_R - \Gamma_L)G^R(f_L \Gamma_L + f_R \Gamma_R)G^A] \quad (156)$$

$$\begin{aligned} &= \frac{e}{2} \int \frac{d\omega}{2\pi} \text{Tr} [-f_L \Gamma_L G^R \Gamma_L G^A - f_L \Gamma_L G^R \Gamma_R G^A + f_R \Gamma_R G^R \Gamma_L G^A + f_R \Gamma_R G^R \Gamma_R G^A \\ &\quad + f_L \Gamma_L G^R \Gamma_L G^A - f_L \Gamma_R G^R \Gamma_L G^A + f_R \Gamma_L G^R \Gamma_R G^A - f_R \Gamma_R G^R \Gamma_R G^A] \end{aligned} \quad (157)$$

$$= -\frac{e}{2} \int \frac{d\omega}{2\pi} \text{Tr} [(f_L - f_R)(\Gamma_L G^R \Gamma_R G^A) + (f_L - f_R)(\Gamma_R G^R \Gamma_L G^A)] \quad (158)$$

$$= -\frac{e}{2\pi} \int d\omega \text{Tr} [(f_L - f_R)(\Gamma_L G^R \Gamma_R G^A)] \quad (159)$$

Now \hbar was 1. correct prefactor, $e/(2\pi) \rightarrow e/(\hbar 2\pi) = e/h$

The prefactor in the definition of the current in the tight binding scheme (eq.(113)) is imaginary, but the evaluated current is real.

7 surface Green function, non-orthogonal basis

7.1 normal

$$(\omega S - H)G = 1 \quad (160)$$

$$H = \begin{bmatrix} H_{00} & H_{01} & 0 & 0 & 0 \\ H_{10} & H_{11} & H_{12} & 0 & 0 \\ 0 & H_{21} & H_{22} & H_{23} & 0 \\ 0 & 0 & H_{32} & H_{33} & \ddots \\ 0 & 0 & 0 & \ddots & \ddots \end{bmatrix} \quad (161)$$

$$S = \begin{bmatrix} S_{00} & S_{01} & 0 & 0 & 0 \\ S_{10} & S_{11} & S_{12} & 0 & 0 \\ 0 & S_{21} & S_{22} & S_{23} & 0 \\ 0 & 0 & S_{32} & S_{33} & \ddots \\ 0 & 0 & 0 & \ddots & \ddots \end{bmatrix} \quad (162)$$

$$G = \begin{bmatrix} G_{00} & G_{01} & G_{02} & G_{13} & \ddots \\ G_{10} & G_{11} & G_{12} & & \\ G_{21} & G_{21} & G_{22} & & \\ G_{31} & & & G_{33} & \\ \vdots & & & & \ddots \end{bmatrix} \quad (163)$$

Use G_{i0} column,

$$(\omega S_{00} - H_{00})G_{00} + (\omega S_{01} - H_{01})G_{10} = I \quad (164)$$

$$(\omega S_{10} - H_{10})G_{00} + (\omega S_{11} - H_{11})G_{10} + (\omega S_{12} - H_{12})G_{20} = 0 \quad (165)$$

$$(\omega S_{21} - H_{21})G_{10} + (\omega S_{22} - H_{22})G_{20} + (\omega S_{23} - H_{23})G_{30} = 0 \quad (166)$$

$$\vdots \quad (167)$$

The last two eqs are generalized as

$$(\omega S_{nn} - H_{nn})G_{n0} = -(\omega S_{n,n-1} - H_{n,n-1})G_{n-1,0} - (\omega S_{n,n+1} - H_{n,n+1})G_{n+1,0} \quad (168)$$

rewrite the relation between the neighboring site.

$$g_{s0}^{-1}G_{00} = I + \alpha_0 G_{10} \quad (169)$$

$$g_0^{-1}G_{n0} = \beta_0 G_{n-1,0} + \alpha_0 G_{n+1,0} \quad (170)$$

The relationship between the second neighboring is

$$g_{s0}^{-1}G_{00} = I + \alpha_0 g_0 (\beta_0 G_{0,0} + \alpha_0 G_{2,0})$$

$$(g_{s0}^{-1} - \alpha_0 g_0 \beta_0)G_{00} = I + \alpha_0 g_0 \alpha_0 G_{2,0}$$

$$g_{s1}^{-1}G_{00} = I + \alpha_1 G_{20} \quad (171)$$

And

$$g_0^{-1}G_{n0} = \beta_0 g_0 (\beta_0 G_{n-2,0} + \alpha_0 G_{n,0}) \\ + \alpha_0 g_0 (\beta_0 G_{n,0} + \alpha_0 G_{n+2,0})$$

$$\{g_0^{-1} - \beta_0 g_0 \alpha_0 - \alpha_0 g_0 \beta_0\}G_{n0} = \beta_0 g_0 \beta_0 G_{n-2,0} + \alpha_0 g_0 \alpha_0 G_{n+2,0} \quad (172)$$

$$g_1^{-1}G_{n0} = b_1 G_{n-2,0} + \alpha_1 G_{n+2,0} \quad (173)$$

the relation between 2^i th neighboring layer is

$$g_{si}^{-1}G_{00} = I + \alpha_i G_{2^i,0} \quad (174)$$

$$g_i^{-1}G_{n0} = \beta_i G_{n-2^i,0} + \alpha_i G_{n+2^i,0} \quad (175)$$

$g_{si}, g_i, \alpha_i, \beta_i$ can be evaluated iteratively

$$g_{s,i+1}^{-1} = g_{s,i}^{-1} - \alpha_i g_i \beta_i \quad (176)$$

$$g_{i+1}^{-1} = g_i^{-1} - \beta_i g_i \alpha_i - \alpha_i g_i \beta_i \quad (177)$$

$$a_{i+1} = \alpha_i g_i \alpha_i \quad (178)$$

$$b_{i+1} = \beta_i g_i \beta_i \quad (179)$$

especially

$$G_{00} = g_{s,i}|_{i \rightarrow \infty} \quad (180)$$

7.2 use transfer matrix

$$G_{n0} = t_0 G_{n-1,0} + \tilde{t}_0 G_{n+1,0} \quad (181)$$

$$t_0 = -(\omega S_{00} - H_{00})^{-1}(\omega S_{01}^\dagger - H_{01}^\dagger) \quad (182)$$

$$\tilde{t}_0 = -(\omega - H_{00})^{-1}(\omega S_{01} - H_{01}) \quad (183)$$

$$G_{10} = T G_{00} \quad (184)$$

where $T = T_i|_{i \rightarrow \infty}$

$$(\omega S_{00} - H_{00})G_{00} + (\omega S_{01} - H_{01})T G_{00} = I \quad (185)$$

$$G_{00} = \{\omega S_{00} - H_{00} + (\omega S_{01} - H_{01})T\}^{-1} \quad (186)$$

8 block matrix, non-orthogonal basis

$$(\omega S - H)G = I$$

consider L,C and R region and rewrite it

$$(\omega S - H) = \begin{bmatrix} \omega S_L - H_L & \omega S_{LC} - H_{LC} & 0 \\ \omega S_{CL} - H_{CL} & \omega - H_C & \omega S_{CR} - H_{CR} \\ 0 & \omega S_{RC} - H_{RC} & \omega S_R - H_R \end{bmatrix} \quad (187)$$

$$G_C = [\omega S_C - H_C - (\omega S_{CR} - H_{CR})(\omega - H_R)^{-1}(\omega S_{RC} - H_{RC}) - (\omega S_{CL} - H_{CL})(\omega - H_L)^{-1}(\omega S_{LC} - H_{LC})]^{-1} \quad (188)$$

$$= \{\omega S_C - H_C - \Sigma_R - \Sigma_L\}^{-1} \quad (189)$$

$$\Sigma_R = (\omega S_{CR} - H_{CR})(\omega S_R - H_R)^{-1}(\omega S_{RC} - H_{RC}) \quad (190)$$

$$\Sigma_L = (\omega S_{CL} - H_{CL})(\omega S_L - H_L)^{-1}(\omega S_{LC} - H_{LC}) \quad (191)$$

9 $\rho \rightarrow V_H$

From Hirose and Tsukada PRB. 51, 5278 (1995) and Hirose's thesis[4, 5].

How to solve

$$\nabla^2 V_H(r) = -4\pi\rho(r) \quad (192)$$

when $V_H(x, y, z = z_0)$ and $V_H(x, y, z = z_{l+1})$ are given.

change the coordinate $r = (x, y, z) \rightarrow (G_{\parallel}, z)$, where $G_{\parallel} = (G_x, G_y)$.

$$V_H(r) = \sum_{G_{\parallel}} V_H(G_{\parallel}, z) e^{iG_{\parallel} r_{\parallel}} \quad (193)$$

$$\rho(r) = \sum_{G_{\parallel}} \rho(G_{\parallel}, z) e^{iG_{\parallel} r_{\parallel}} \quad (194)$$

$$\left(\frac{d^2}{dz^2} - G_{\parallel}^2 \right) V_H(G_{\parallel}, z) = -4\pi\rho(G_{\parallel}, z) \quad (195)$$

Introduce a Green function

$$\left(\frac{d^2}{dz^2} - G_{\parallel}^2\right)G(G_{\parallel}, z, z') = -\delta(z, z') \quad (196)$$

$$G(G_{\parallel}, z) = \int dk G(G_{\parallel}, k) e^{ikz} \quad (197)$$

9.1 the case of $G_{\parallel} \neq 0$

Let's solve G with the boundary conditon, $G(z = z_0, z') = 0$ and $G(z = z_{l+1}, z') = 0$. First the solution in the free condition is.

$$G(G_{\parallel}, k) = 1/(G_{\parallel}^2 + k^2) \quad (198)$$

$$G(G_{\parallel}, z) = \int dk e^{ikz} \frac{1}{G_{\parallel}^2 + k^2} \quad (199)$$

$$= \begin{cases} \frac{2\pi i}{2\pi} \frac{e^{-|G_{\parallel}|z}}{2i|G_{\parallel}|} = \frac{e^{-|G_{\parallel}|z}}{2|G_{\parallel}|}, (z > 0) \\ \frac{e^{|G_{\parallel}|z}}{2|G_{\parallel}|}, (z < 0) \end{cases} \quad (200)$$

Next, G with the boundary conditon, $G(z = z_0, z') = 0$ and $G(z = z_{l+1}, z') = 0$, G can be solved by applying a method of images

$$G(G_{\parallel}, z, z') = \frac{e^{-G|z-z'|} + e^{-G(2(z_{l+1}-z_0)-|z-z'|)} - e^{-G(2z_{l+1}-z-z')} - e^{-G(z+z'-2z_0)}}{2G(1 - e^{-2G(z_{l+1}-z_0)})} \quad (201)$$

where $G = |G_{\parallel}|$.

Green's theorem

$$\int_S dS' n \cdot (u \nabla v - v \nabla u) = \int_V dV' (u \Delta v - v \Delta u) \quad (202)$$

can be read in this case, when $V_H(z_0)$ and $V_H(z_{l+1})$ are given,

$$[G(z, z') \partial_{z'} V_H(z') - V_H(z') \partial_{z'} G(z, z')]_{z_0}^{z_{l+1}} \quad (203)$$

$$= \int dz' (G(z, z') \partial_{z'}^2 V_H(z') - V_H(z') \partial_{z'}^2 G(z, z')) \quad (204)$$

$$= \int dz' \left(G(z, z') (G_{\parallel}^2 V_H(z') - 4\pi \rho(z')) - V_H(z') (G_{\parallel}^2 G(z, z') - \delta(z - z')) \right) \quad (205)$$

$$= -4\pi \int_{z_0}^{z_{l+1}} dz' G(z, z') \rho(z') + V_H(z) \quad (206)$$

Thus

$$V_H(z) = 4\pi \int_{z_0}^{z_{l+1}} dz' G(z, z') \rho(z') + [G(z, z') \partial_{z'} V_H(z') - V_H(z') \partial_{z'} G(z, z')]_{z_0}^{z_{l+1}} \quad (207)$$

$$= 4\pi \int_{z_0}^{z_{l+1}} dz' G(z, z') \rho(z') - [V_H(z') \partial_{z'} G(z, z')]_{z'=z_0}^{z'=z_{l+1}} \quad (208)$$

$$\begin{aligned} V_H(G_{\parallel}, z) &= 4\pi \int_{z_0}^{z_{l+1}} dz' G(G_{\parallel}, z, z') \rho(G_{\parallel}, z') \\ &+ \left\{ V_H(G_{\parallel}, z_{l+1}) \left(e^{-G(z_{l+1}-z)} - e^{-G(z_{l+1}-2z_0+z)} \right) \right. \\ &+ \left. V_H(G_{\parallel}, z_0) \left(e^{-G(z-z_0)} - e^{-G(2z_{l+1}-z_0-z)} \right) \right\} / \left(1 - e^{-2G(z_{l+1}-z_0)} \right) \end{aligned} \quad (209)$$

$$\begin{aligned}
&= 4\pi \int dk \frac{\rho(G_{\parallel}, k)}{G^2 + k^2} e^{ikz} \\
&\quad + \left\{ V_H(G_{\parallel}, z_{l+1}) \left(e^{-G(z_{l+1}-z)} - e^{-G(z_{l+1}-2z_0+z)} \right) \right. \\
&\quad \left. + V_H(G_{\parallel}, z_0) \left(e^{-G(z-z_0)} - e^{-G(2z_{l+1}-z_0-z)} \right) \right\} / \left(1 - e^{-2G(z_{l+1}-z_0)} \right) \\
V_H(r) &= 4\pi \int dk \frac{\rho(G_{\parallel}, k)}{G^2 + k^2} e^{i(G_{\parallel}r_{\parallel} + kz)} \\
&\quad + \int dG_{\parallel} e^{iG_{\parallel}r_{\parallel}} \left\{ V_H(G_{\parallel}, z_{l+1}) \left(e^{-G(z_{l+1}-z)} - e^{-G(z_{l+1}-2z_0+z)} \right) \right. \\
&\quad \left. + V_H(G_{\parallel}, z_0) \left(e^{-G(z-z_0)} - e^{-G(2z_{l+1}-z_0-z)} \right) \right\} / \left(1 - e^{-2G(z_{l+1}-z_0)} \right) \quad (210)
\end{aligned}$$

Note that $\rho(G, z_0) = 0$ and $\rho(G, z_{l+1}) = 0$. Thus the Fourier transform of $\rho(G, z)$ is executed in the region from z_1 to z_l .

$V_H(G_{\parallel} \neq 0, z_0) = 0$ and $V_H(G_{\parallel} \neq 0, z_{l+1}) = 0$ when the left and right electrodes are jellium.

9.2 the case of $G_{\parallel} = 0$

9.2.1 solve iteratively

$$\frac{d^2}{dz^2} V_H^0(z) = -4\pi \rho^0(z) \quad (211)$$

where $V_H^0(z) = V_H(G_{\parallel} = 0, z)$ and $\rho^0(z) = \rho(G_{\parallel} = 0, z)$. The above equation is equivalent to

$$\left(\frac{d^2}{dz^2} - K^2 \right) V_H^0(z) = -4\pi \rho^0(z) - K^2 V_H^0(z) \quad (212)$$

with arbitrary K . Using the Green function $G(K, z, z')$ with the boundary condition $G(K, z = z_0, z') = 0$ and $G(K, z = z_{l+1}, z') = 0$ (same as eq.(201))

$$V_H^0(z) = \int_{z_0}^{z_{l+1}} dz' G(K, z, z') \left(4\pi \rho^0(z') + K^2 V_H^0(z') \right) - [V_H(z') \partial_{z'} G(K, z, z')]_{z'=z_0}^{z'=z_{l+1}} \quad (213)$$

It seems that eq.(213) is especially stable to solve $V_H^0(z)$ iteratively. Nara-san says that a few of iterations are enough to converge V_H^0 .

9.2.2 solve directly

An alternative way to solve eq. (211) (Kobayashi's method)

$$\frac{d}{dz} V_H^0(z) = -4\pi \int_{z_0}^z dz' \rho^0(z') + a \quad (214)$$

$$V_H^0(z) = -4\pi \int_{z_0}^z dz'' \int_{z_0}^{z''} dz' \rho^0(z') + a(z - z_0) + b \quad (215)$$

$$= \Delta_2(z) + a(z - z_0) + b \quad (216)$$

where a and b are some constants. They can be determined from the he boundary conditions

$$V_H^0(z_0) = \Delta_2(z_0) + b = b \quad (217)$$

$$V_H^0(z_{l+1}) = \Delta_2(z_{l+1}) + a(z_{l+1} - z_0) + b \quad (218)$$

Nara-san says that when the z -mesh is fine enough, the latter method with a simple integration scheme to evaluate Δ_2 gives almost the same precision as the former method.

10 $\rho \rightarrow V_H$, another (easier) derivation

10.1 add boundary condition without any charge

How to solve

$$\nabla^2 V_H(r) = -4\pi\rho(r) \quad (219)$$

when $V_H(x, y, z = z_0)$ and $V_H(x, y, z = z_{l+1})$ are given.

split $V_H(r) = \phi(r) + \psi(r)$,

$$\nabla^2 \phi(r) = -4\pi\rho(r) \quad (220)$$

$$\nabla^2 \psi(r) = 0 \quad (221)$$

$$\nabla^2(\phi(r) + \psi(r)) = -4\pi\rho(r) \quad (222)$$

where $\phi(r)$ is the solution of the Poisson equation with charge $\rho(r)$ without any boundary condition in the region from $z = z_1$ to $z = z_l$. $\psi(r)$ is the solution of the Poisson equation without charge and with the boundary condition $V_H(x, y, z = z_0)$ and $V_H(x, y, z = z_{l+1})$ in the region from $z = z_0$ to $z = z_{l+1}$.

$\phi(G)$, the Fourier transform of $\phi(r)$, can be solved in the usual way for periodic boundary condition as

$$\phi(G) = 4\pi\rho(G)/G^2 \quad (223)$$

$\psi(G_{\parallel}, z)$ can be solved analytically using the formula of the previous chapter with the condition $\rho = 0$. Surely eq.(210) has such a form. $\psi(G_{\parallel} = 0, z)$ can be also solved using the formula of the previous chapter with the condition $\rho^0 = 0$. The solution, eq(221), is simply,

$$\psi(r) = (\mu_R - \mu_L)/(z_{l+1} - z_0) \quad (224)$$

10.2 meanings of the excess charge

How to solve

$$\nabla^2 V_H(r) = -4\pi\rho(r) \quad (225)$$

when $V_H(x, y, z = z_0)$ and $V_H(x, y, z = z_{l+1})$ are given.

Define a parameter, which means the excess charge,

$$\rho_B = \rho(r) - \sum_{G \neq 0} \rho(G) \quad (226)$$

Then

$$\nabla^2(V(r) + V_B(r)) = -4\pi(\rho(r) + \rho_B) \quad (227)$$

$$\nabla^2 V(r) = -4\pi\rho(r) \quad (228)$$

$$\nabla^2 V_B(r) = -4\pi\rho_B \quad (229)$$

$$(230)$$

Eq.(228) is solved via FFT, while Eq.(229) is solved analytically,

$$V_B(z) = -4\pi\rho_B(z - z_0)^2 + a(z - z_0) + b \quad (231)$$

parameter a and b is determined via boundary condition. The sign of ρ_B determines how $V_H(z)$ drops. (See figure.1.)

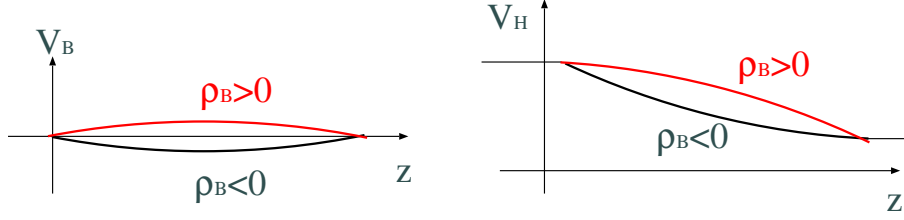
Note that the condition of no s-d bias voltage is satisfied, even if there exists some excess charge,

11 some examples

11.1 an 1D chain

Consider a tight binding model,

$$H = \sum_{\langle ij \rangle} t c_i c_j \quad (232)$$

Figure 1: relationship between ρ_B and $V(z)$

11.1.1 If site 0 is in the central region

Assume that

$$\Sigma_R(\omega^-) = \omega_0/2 + i\Gamma_0/2 \quad (233)$$

where $\omega^\pm = \omega \pm i\delta$.

$$G_C = (\omega - \Sigma_R - \Sigma_L) \quad (234)$$

$$\Sigma_R(\omega^-) = \text{Re}\Sigma_R + i\text{Im}\Sigma_R = \omega_0/2 + i\Gamma_0/2 \quad (235)$$

$$\Sigma_R(\omega^+) = \text{Re}\Sigma_R - i\text{Im}\Sigma_R = \omega_0/2 - i\Gamma_0/2 \quad (236)$$

$$\Gamma = \text{Im}(\Sigma_R(\omega^-) - \Sigma_R(\omega^+)) = \Gamma_0 \quad (237)$$

Then

$$G_C(\omega^+) = 1/(\omega - \omega_0 - i\Gamma_0) \quad (238)$$

conductance is

$$T = \Gamma G_C(\omega^+) \Gamma G_C(\omega^-) \quad (239)$$

$$= \Gamma_0^2 / ((\omega - \omega_0)^2 + \Gamma_0^2) \quad (240)$$

where ω_0 and Γ_0 are functions of ω and must be calculated. $\omega_0 = \omega$ in the range from $-2t$ to $2t$ also from numerical calculations. Therefore $T = 1$ from $\omega = -2t$ to $\omega = 2t$, and $G_C = 1/(-i\Gamma_0)$.

11.1.2 If site0 and site1 are in the central region

Matrixes for site0 and site1 are

$$H = \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix} \quad (241)$$

$$\Sigma_L(\omega^-) = \begin{pmatrix} \omega_0/2 + i\Gamma_0/2 & 0 \\ 0 & 0 \end{pmatrix} \quad (242)$$

$$\Sigma_R(\omega^-) = \begin{pmatrix} 0 & 0 \\ 0 & \omega_0/2 + i\Gamma_0/2 \end{pmatrix} \quad (243)$$

$$\Gamma_L = \begin{pmatrix} \Gamma_0 & 0 \\ 0 & 0 \end{pmatrix} \quad (244)$$

$$\Gamma_R = \begin{pmatrix} 0 & 0 \\ 0 & \Gamma_0 \end{pmatrix} \quad (245)$$

$$G_C(\omega^+) = (\omega - H - \Sigma_R(\omega^+) - \Sigma_L(\omega^+))^{-1} \quad (246)$$

Then

$$T = \text{Tr}[\Gamma_L G_C(\omega^+) \Gamma_R G_C(\omega^-)] \quad (247)$$

$$= \frac{16\Gamma_0^2 t^2}{(\Gamma_0^2 + (2t + \omega)^2)(\Gamma_0^2 + (2t - \omega)^2)} \quad (248)$$

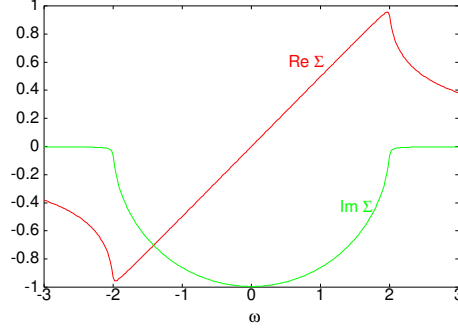


Figure 2: Self-energy of surface Green function of the simple tight binding model of eq.(232) at $t = 1$. A figure shows a result of numerical calculation of $\Sigma(\omega + i\delta)$ where $\delta = 0.01$.

where $\omega_0 = \omega$ is used. $T = 1$ also in this case. Then

$$\Gamma_0 = \sqrt{4t^2 - \omega^2} \quad (249)$$

A numerical calculation supports this result.

In summary, self-energy of the surface Green function of the simple tight-binding model is

$$\Sigma_{R \text{ or } L}(\omega^\pm) = \frac{\omega}{2} \mp i \frac{\sqrt{4t^2 - \omega^2}}{2} \quad (250)$$

for $-2t < \omega < 2t$.

11.2 an 1D chain with an impurity — a dip structure

11.2.1 an impurity interacting with a atom

$$H = \sum_{\langle ij \rangle} tc_i c_j + fd_0^+ d_0 + (sc_0^+ d_0 + \text{h.c.}) \quad (251)$$

If site 0 is in the central region, matrixes for the site of c_0 and d_0 are

$$G_C(\omega^+) = \begin{pmatrix} \omega - \Sigma_R(\omega^+) - \Sigma_L(\omega^+) & -s \\ -s & \omega - f \end{pmatrix}^{-1} \quad (252)$$

$$= \begin{pmatrix} \omega - \omega_0 + i\Gamma_0 & -s \\ -s & \omega - f \end{pmatrix}^{-1} \quad (253)$$

$$G_C(\omega^-) = \begin{pmatrix} \omega - \omega_0 - i\Gamma_0 & -s \\ -s & \omega - f \end{pmatrix}^{-1} \quad (254)$$

$$\Gamma_R = \begin{pmatrix} \Gamma_0 & 0 \\ 0 & 0 \end{pmatrix} \quad (255)$$

$$\Gamma_L = \begin{pmatrix} \Gamma_0 & 0 \\ 0 & 0 \end{pmatrix} \quad (256)$$

$$T = \text{Tr} [\Gamma_L G_C(e^+) \Gamma_R G_C(e^-)] \quad (257)$$

$$= \frac{\Gamma_0^2 (\omega - f)^2}{\{(\omega - f)(\omega - \omega_0) - s^2\}^2 + \Gamma_0^2 (\omega - f)^2} \quad (258)$$

$$= \frac{\Gamma_0^2 (\omega - f)^2}{s^4 + \Gamma_0^2 (\omega - f)^2} \quad (259)$$

where $\omega_0 = \omega$ is used at the last equality. It is important to notice that $T = 0$ at $\omega = f$, i.e. at the energy level of the impurity and the maximum is less than 1. The half-width of the minimum is s^2/Γ_0 .

11.2.2 an impurity interacting with two atoms

$$H = \sum_{\langle ij \rangle} tc_i c_j + fd_0^\dagger d_0 + (sc_0^\dagger d_0 + sc_1^\dagger d_0 + \text{h.c.}) \quad (260)$$

The conductance of this model is calculated as

$$T = \frac{16\Gamma_0^2(s^2 - ft + tw)^2}{(\Gamma_0^2 + (2t + \omega)^2)(f^2\Gamma_0^2 + (4s^2 - 2ft + f\omega - \Gamma_0\omega + 2t\omega - w^2)^2)} \quad (261)$$

A position of a dip structure is not necessarily at $\omega = f$. The dip appears at $\omega = f - s^2/t$ in this case.

11.3 junction — a resonance peak

$$H = \sum_{\langle ij \rangle \neq 0} tc_i^\dagger c_j + fc_0^\dagger c_0 + (sc_1^\dagger c_0 + sc_{-1}^\dagger c_0 + \text{h.c.}) \quad (262)$$

Only site 0 is in the central region. Because $\Sigma_R(\omega) = H_{CR}G_R(\omega)H_{RC}$ and s enters only through H_{CR} and H_{RC} ,

$$\Sigma_R(\omega) = (s/t)^2 \Sigma_{R0}(\omega) \quad (263)$$

where Σ_{R0} is the value of Σ_R when $s = t$. Then

$$G = (\omega - (s/t)^2\omega_0 - i(s/t)^2\Gamma_0 - f)^{-1} \quad (264)$$

$$T = \frac{(s/t)^4\Gamma_0^2}{(\omega - (s/t)^2\omega_0 - f)^2 + (s/t)^4\Gamma_0^2} \quad (265)$$

$$= \frac{\frac{(s/t)^4\Gamma_0^2}{(1-(s/t)^2)^2}}{\left(\omega - \frac{f}{1-(s/t)^2}\right)^2 + \frac{(s/t)^4\Gamma_0^2}{(1-(s/t)^2)^2}} \quad (266)$$

$T = 1$ at the center of the peak, $\frac{f}{1-(s/t)^2}$, and the half-width of the maximum is $\frac{\Gamma_0(s/t)^2}{1-(s/t)^2}$. Smaller s , and smaller Γ_0 , which means smaller t or the energy is near the edge of the band, give a shaper resonance peak on the conductance.

T takes some value, $\Gamma_0^2/(\Gamma_0^2 + f^2)$ for $s = t$. (Γ_0 is a function of ω .) The broad peak locates not at $\omega = f$, but at $\omega = 0$, which is the center of the band.

A H^{-1}

$$G = \begin{pmatrix} E - H_A & -H_{AB} \\ -H_{BA} & E - H_B \end{pmatrix}^{-1} \quad (267)$$

$$= \begin{pmatrix} \frac{1}{E - H_A - H_{AB} \frac{1}{E - H_B} H_{BA}} & -\frac{1}{E - H_A} H_{AB} \frac{1}{E - H_B - H_{BA} \frac{1}{E - H_A} H_{AB}} \\ -\frac{1}{E - H_B} H_{BA} \frac{1}{E - H_A - H_{AB} \frac{1}{E - H_B} H_{BA}} & \frac{1}{E - H_B - H_{BA} \frac{1}{E - H_A} H_{AB}} \end{pmatrix} \quad (268)$$

B phase between the neighbouring site

The formula (128) can be used to calculate the current of the link ij , $J_L(t)_{ij}$,

$$J_L(t) = \sum_{ii} J_L(t)_{ij} \quad (269)$$

$$J_L(t)_{ij} = 2e \text{Re} [t_{ij} G_{ji}^<(t, t)] \quad (270)$$

The wavefunction, Ψ , is solved in the time-independent non-equilibrium state. The charge at (r, E) is calculated as

$$n(r, E) = \Psi^*(r, E)\Psi(r, E) \quad (271)$$

while

$$n(r, E) = \frac{1}{2\pi i} G^<(r, E) \quad (272)$$

The total charge is $n(r) = \int dE n(r, E)$. These reads that $\Psi(r, E)^* \Psi(r, E)$ is associated with $1/(2\pi i) G^<(r, E)$. [9]
Then $J_{L,ij}$ is [8]

$$J_{L,ij} = 2e \operatorname{Re} \frac{1}{2\pi} \int dE G^<(r, E) \quad (273)$$

$$= 2e \operatorname{Re} \frac{1}{2\pi} \int dE [t_{ij}(2\pi i) \langle j|E \rangle \langle E|i \rangle] \quad (274)$$

$$= 2e \operatorname{Im} \int dE [t_{ij} \langle j|E \rangle \langle E|i \rangle] \quad (275)$$

$$= 2e \operatorname{Im} \int dE [\langle E|i \rangle t_{ij} \langle j|E \rangle] \quad (276)$$

When $\Psi(E) = \sum_i a_{Ei} \phi_i$, $J_{L,ij} = 2e \int dE t_{ij} |a_{Ei}| |a_{Ej}| \sin(\theta_{Ei} - \theta_{Ej})$, with the phase factor θ_{Ei} of a_{Ei} . This means that no current flows if the phase difference between the site i, j is 0 or π .

Compare it with another definition of the current density

$$j(r) = (1/m^*) \operatorname{Im} [\psi^+(r) \nabla \psi(r)] \quad (277)$$

$\langle E|i \rangle$ in eq.(276) is weight at site i of the wavefunction $\psi(E)$, while $\psi(r)$ is weight at r of the wavefunction. So eq.(276) is similar to eq.(277). (Of course!) if $\psi(r) = \exp(ikr)$, $j(r) = k/m^*$. In this case, $\psi(r + dr) = \exp(ikr) \exp(ik dr)$. Then $\theta = k dr$.

C charge density in the non-orthogonal basis set

In this section, we consider the dual basis representation.

Eigen value and eigen state satisfy the equation,

$$H|\alpha\rangle = E_\alpha|\alpha\rangle$$

$|\alpha\rangle$ is constructed using atomic basis set $|i\rangle$ (LCAO),

$$|\alpha\rangle = \sum_i c_{\alpha,i} |i\rangle$$

The eigen energy is calculated by solving generalized eigenvalue problem,

$$\langle i|H|j\rangle = E \langle i|j\rangle \quad (278)$$

$$H_{ij} = E S_{ij} \quad (279)$$

with the normalization condition $\langle \alpha|\alpha\rangle = 1$. The Green function is defined as

$$G(z) = \sum_\alpha \frac{|\alpha\rangle \langle \alpha|}{z - E_\alpha}$$

Here we define the dual basis set in the atomic basis set,

$$|\bar{i}\rangle = \sum_j |j\rangle S_{ji}^{-1}$$

where $S_{ij} = \langle i|j\rangle$. Then

$$\langle \bar{i}|j\rangle = \delta_{ij}$$

The trace of A is expressed as

$$\operatorname{Tr}[A] = \langle A \rangle = \langle \bar{i}|A|i\rangle$$

The Green function is

$$\langle \bar{i} | G | \bar{j} \rangle = \sum_{\alpha} \frac{\langle \bar{i} | \alpha \rangle \langle \alpha | \bar{j} \rangle}{z - E_{\alpha}} \quad (280)$$

$$= \sum_{\alpha} \frac{c_{\alpha,i} c_{\alpha,j}^*}{z - E_{\alpha}} \quad (281)$$

Then the charge density is

$$\langle \rho \rangle = \sum_i \langle \bar{i} | \rho | i \rangle \quad (282)$$

$$= \sum_{i,j} \langle \bar{i} | \rho | \bar{j} \rangle \langle j | i \rangle \quad (283)$$

$$= \sum_{i,j} \langle \bar{i} | \left\{ - \int dz \frac{1}{\pi} \text{Im} G(z) \right\} | \bar{j} \rangle \langle j | i \rangle \quad (284)$$

$$= - \int dz \frac{1}{\pi} \text{Im} \sum_{i,j} \langle \bar{i} | G(z) | \bar{j} \rangle \langle j | i \rangle \quad (285)$$

$$= - \int dz \frac{1}{\pi} \text{Im} \sum_{i,j} G_{ij} S_{ji} \quad (286)$$

Consider the simple case,

$$\langle \rho \rangle = - \frac{1}{\pi} \text{Im} \int dz \sum_{\alpha, ij} \frac{c_{\alpha i} c_{\alpha j}^*}{z - E_{\alpha} + i\delta} S_{ji} \quad (287)$$

$$= \int dz \sum_{\alpha, ij} c_{\alpha i} c_{\alpha j}^* S_{ji} \delta(z - E_{\alpha}) \quad (288)$$

$$= \sum_{E_{\alpha} \leq E_F} \sum_{ij} c_{\alpha i} c_{\alpha j}^* S_{ji} \quad (289)$$

$$= \sum_{E_{\alpha} \leq E_F} \quad (290)$$

$\sum_{ij} c_{\alpha i} c_{\alpha j}^* S_{ji} = 1$ because of the normalization of $|\alpha\rangle$. The left hand side of $\langle \alpha | \alpha \rangle = 1$ can be written as

$$\langle \alpha | \alpha \rangle = \sum_{ij} (c_{\alpha i}^* \langle i |) (c_{\alpha j} | j \rangle) \quad (291)$$

$$= \sum_{ij} c_{\alpha i}^* c_{\alpha j} S_{ij} \quad (292)$$

The total band energy can be calculated similarly

$$\langle E \rangle = \sum_i \langle \bar{i} | E | i \rangle \quad (293)$$

$$= \sum_i \langle \bar{i} | E | \bar{j} \rangle \langle j | i \rangle \quad (294)$$

$$= \sum_{ij} E_{ij} S_{ji} \quad (295)$$

acknowledgement

Dr. Masato Oda (ver. 2006-04-17)

References

- [1] Quantum Kinetics in Transport and Optics of Semiconductors (Springer Series in Solid State Sciences, 123), H. Haug and A.-P. Jauho.
- [Surface Green function] M.P. López Sancho, et al. J. Phys. F 15, 851 (1965).
- [2] Y. Xue, et al. Chem. Phys. 281, 151 (2002) (condmat/0112136).
- [3] J. Taylor, et al. PRB 63, 245407-1 (2001).
- [TRANSIESTA] M. Grandbyge, et al. PRB 65, 165401-1 (2002).
- [Modified Matsubara summation] D.M.C. Nicholson et al. Phys. Rev. B 50, 14686 (1994).
- [4] K. Hirose and Tsukada PRB. 51, 5278 (1995)
- [5] K. Hirose, thesis
- [6] Y. Meir and N.S. Wingreen, PRL. 68, 2512 (1992).
- [7] N.S. Wingreen, A.-P. Jauho and Y. Meir, PRB. 48, 8487 (1993).
- [8] S. Nakanishi and M. Tsukada, Surf. Sci. 438, 305 (1999).
- [9] Electronic Transport in Mesoscopic Systems (Cambridge University Press, Cambridge Studies in semiconductor Physics and Microelectronic Engineering:3), S. Datta.