Electronic transport calculations by NEGF

- Electronic transport in nano-scale materials:
- Experiments
- Nonequilibrium Green function method
  - From a scattering problem
  - Keldysh method
- Applications
- Usage of OpenMX for the NEGF calculations
- Exercise

Taisuke Ozaki (ISSP, Univ. of Tokyo)

Institute for Materials Research (IMR), Tohoku University, Feb. 14, 2020.

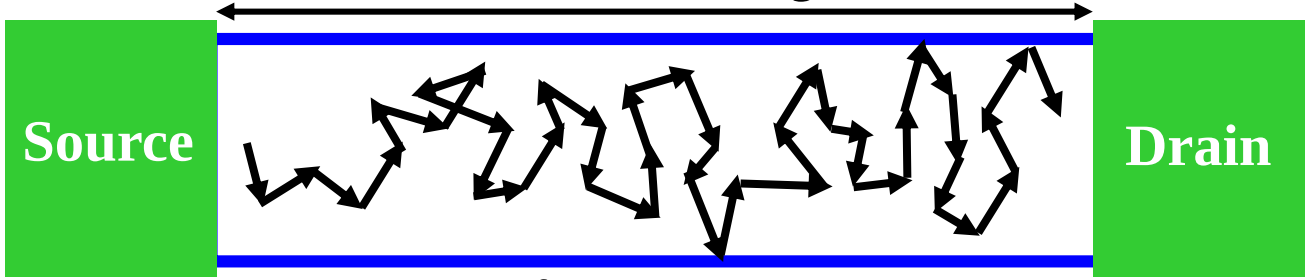
Diffusive/Ballistic transport

λ~20 nm in single crystal Si

Mean free path λ ⟷

Diffusive regime:

Source-drain length L

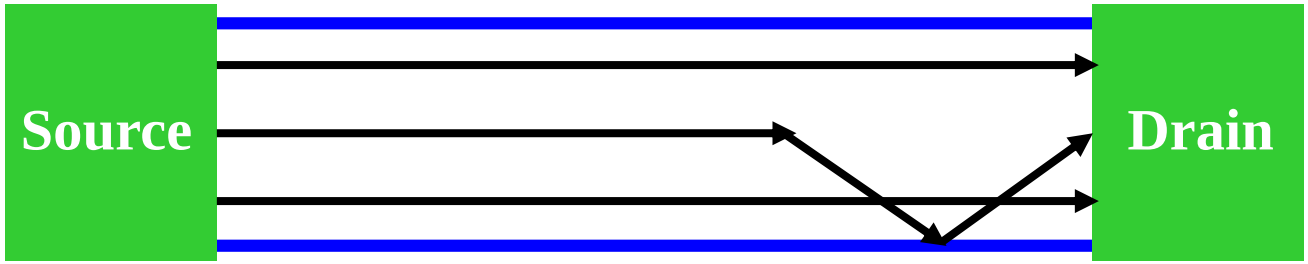


Due to impurity, defect, boundary, e-e int. e-phonon int.

λ<<L

Mobility is important.

Quasi-Ballistic regime:



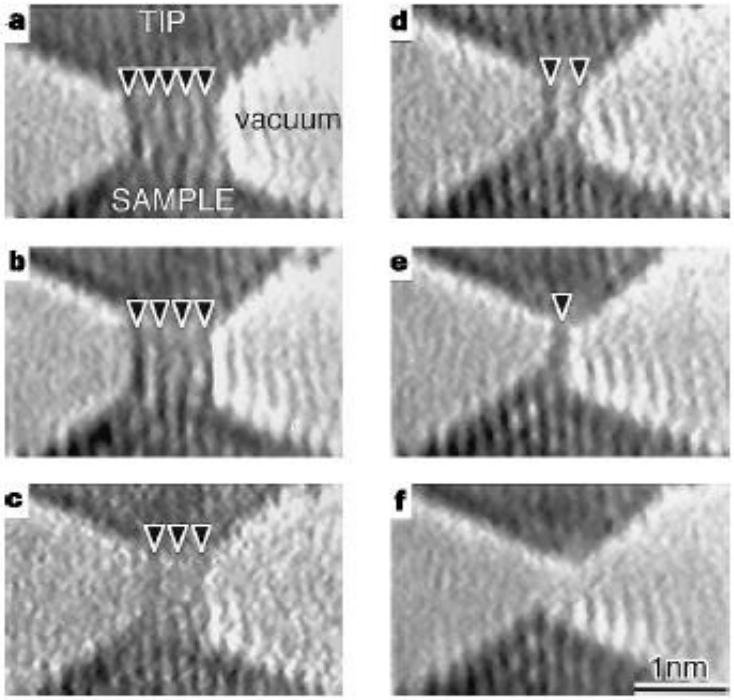
L~λ

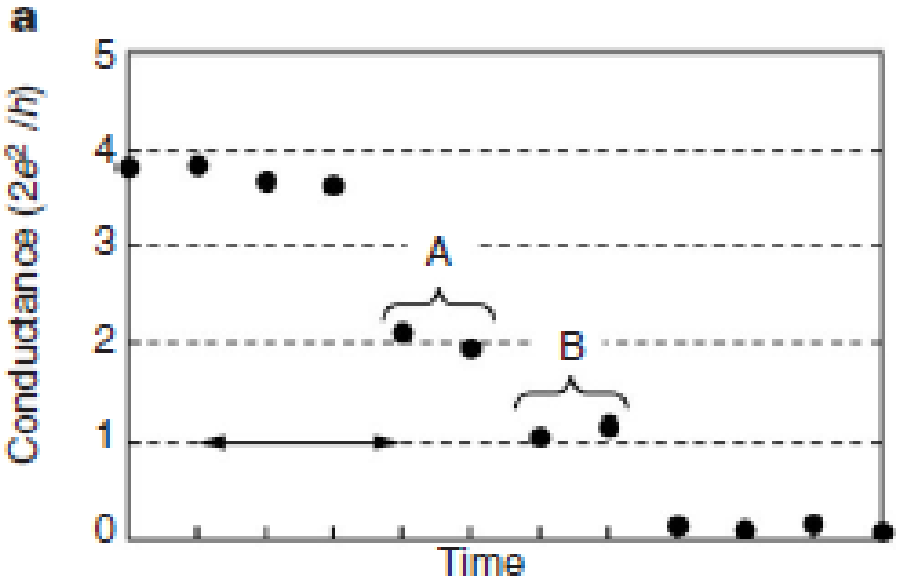
Ballistic regime:

L<λ

Quantum conductance in gold nanowires

After contacting two gold structures, gradually the two strucutres are pulled along the axial direction. Then, the bridging region becomes gradually thinner. Along with the structural change, the conductance changes stepwise.

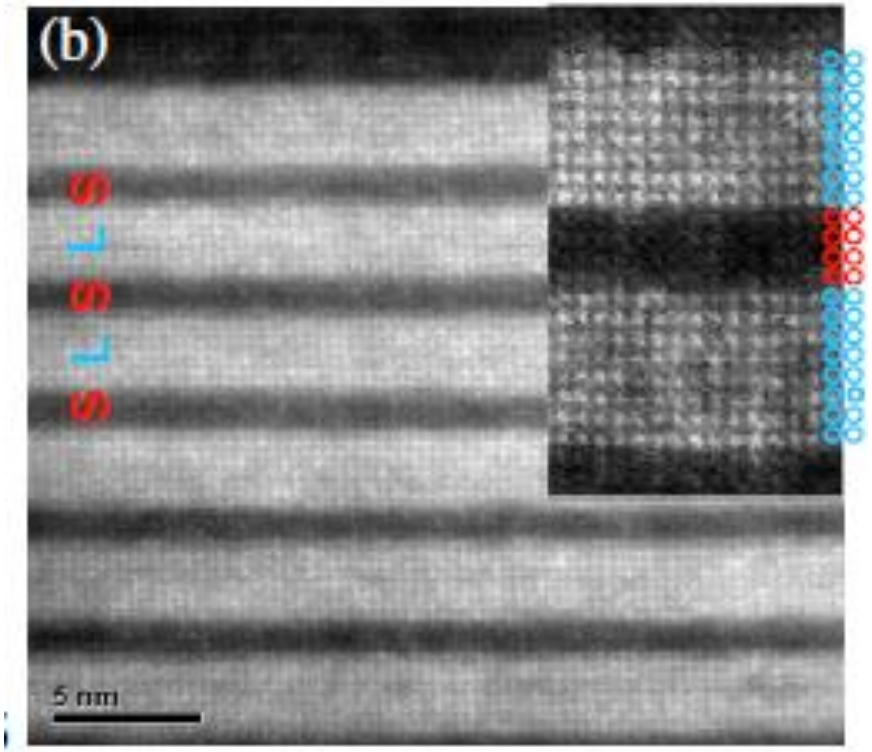


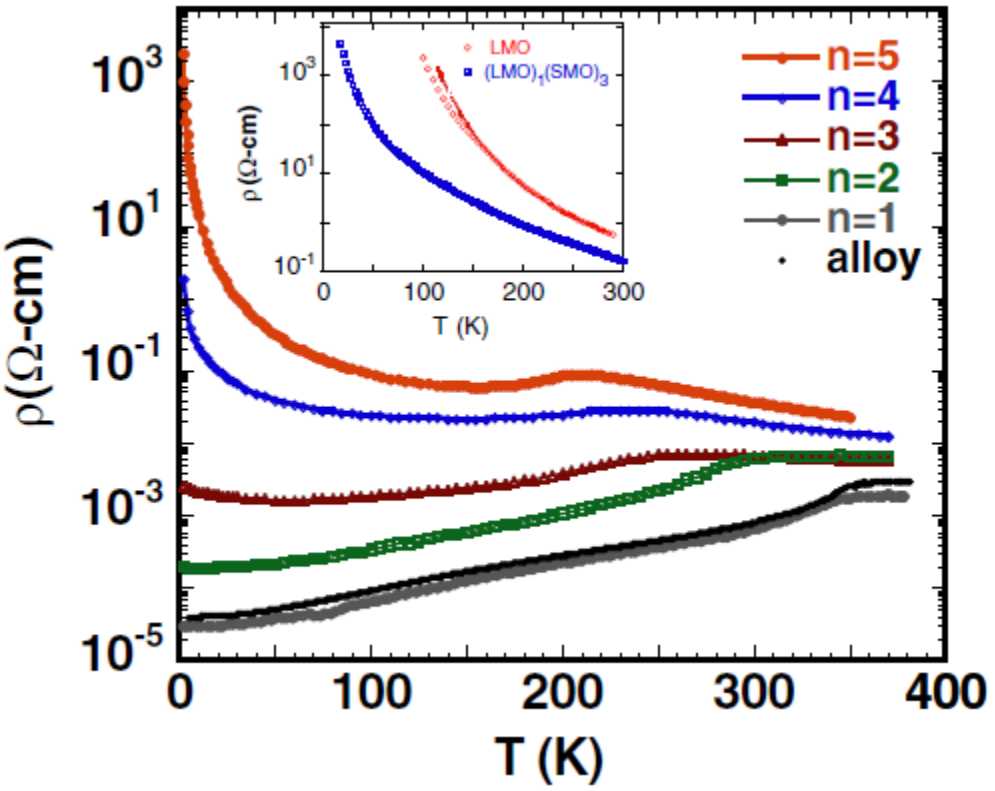


Takayanagi et al., Nature **395**, 780 (1998).

$(LaMnO_3)_{2n}/(SrMnO_3)_n$ superlattice

Depending on the number of layers, the system exhibits a metal-insulator transition. $n<3$ metal, $3 \leqq n$ insulator

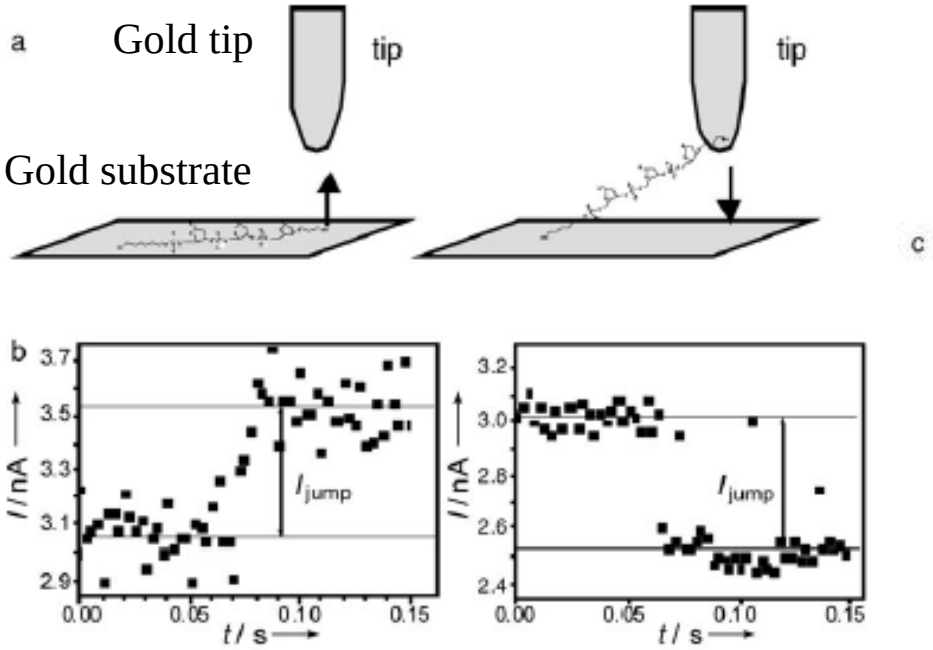




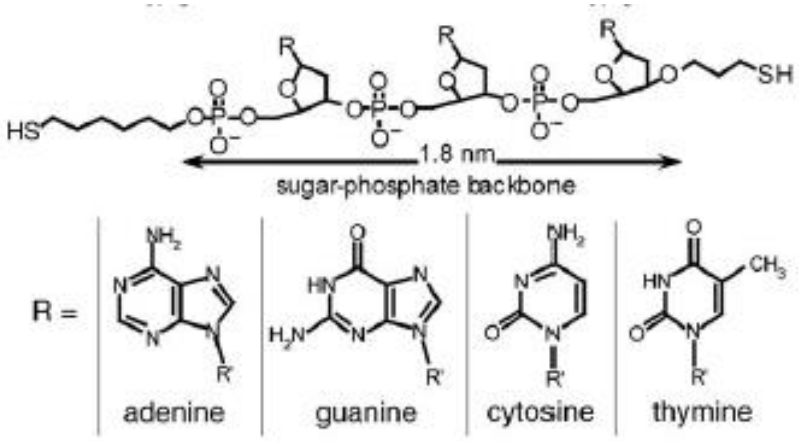
Bhattacharya et al., PRL **100,** 257203 (2008)

Transport in a single strand DNA molecule

Adsorption Detachment



Molecular structure of a single strand DNA molecule

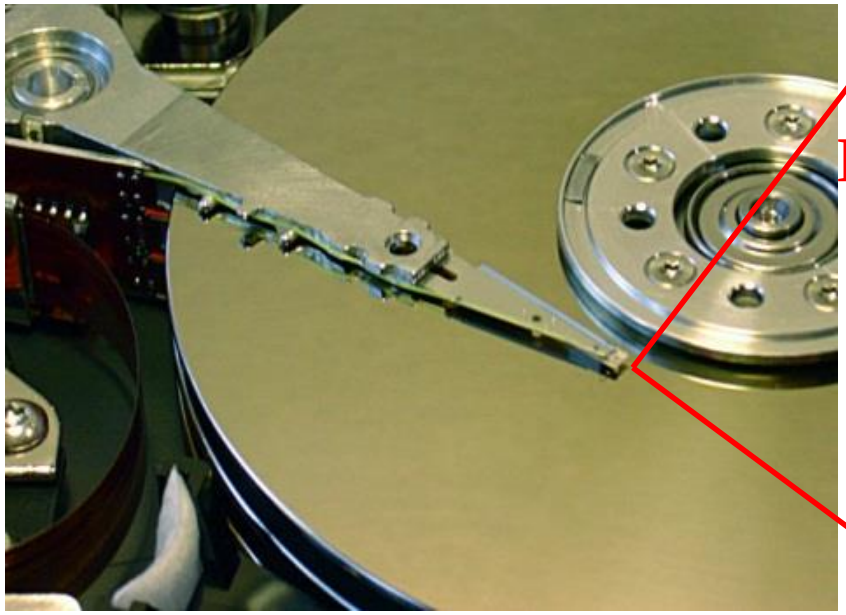


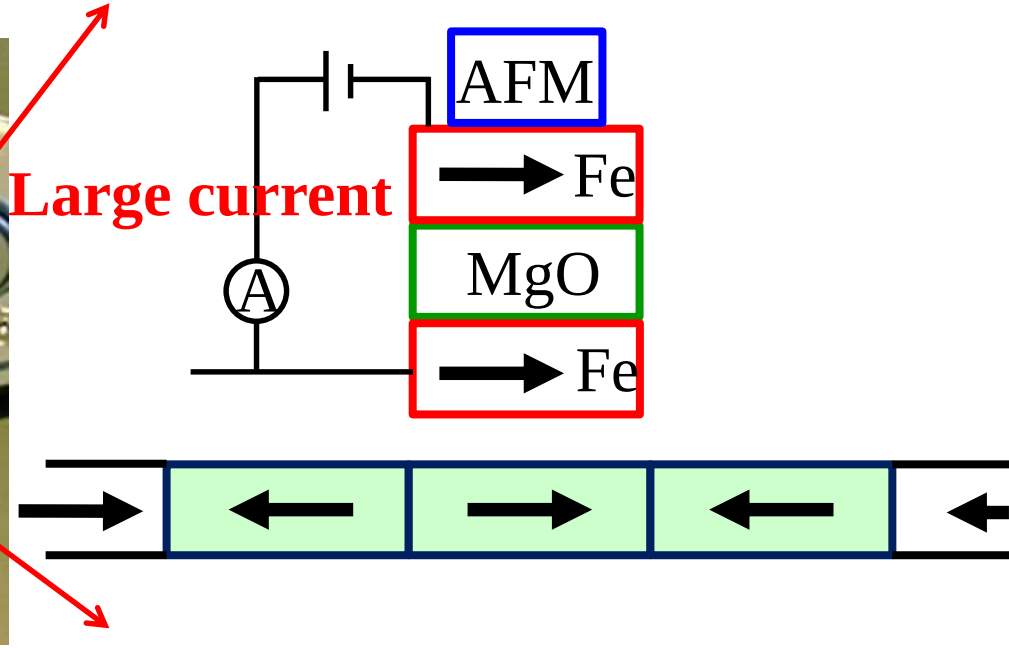
The current jumps when the molecule adsorbs and detaches.

Harm van Zalinge, Chem. Phys. Chem. 7, 94 (2005)

Application of tunneling magnet resistance (TMR) effect

A device used for a hard disk head is based on a tunneling magnet resistance (TMR) effect, in which the tunneling current strongly depends on the relative spin direction of two ferromagnetic regions.





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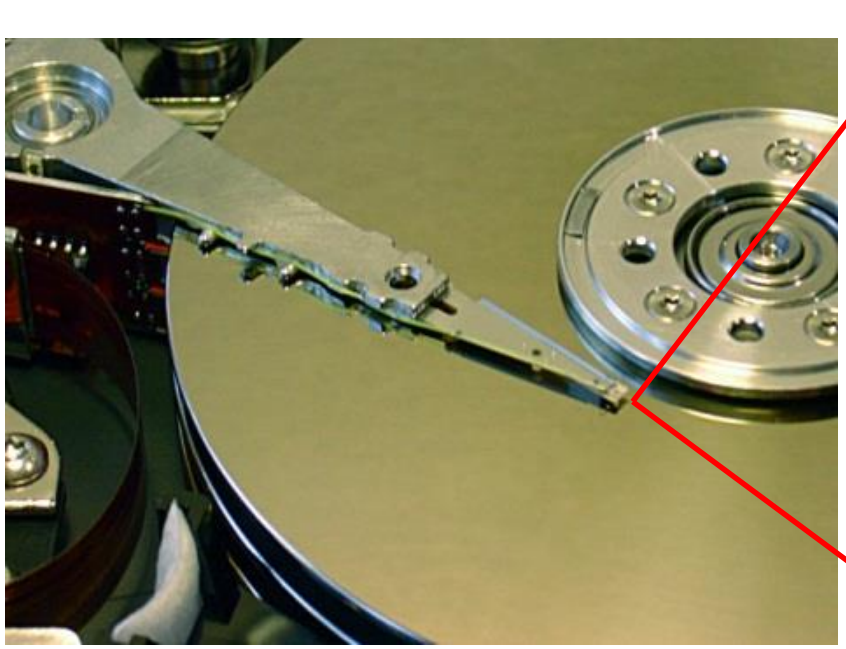
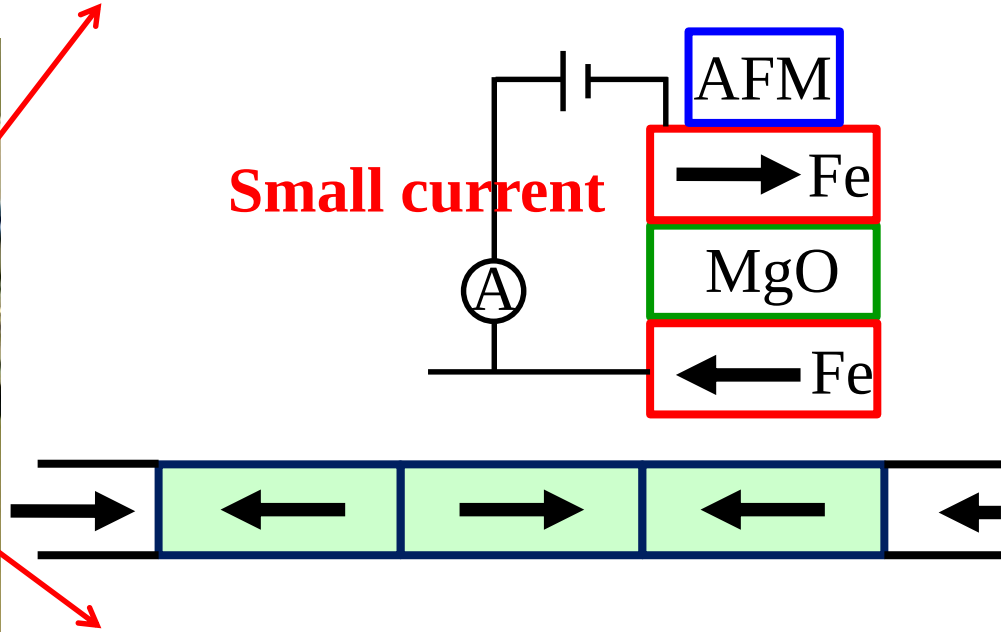
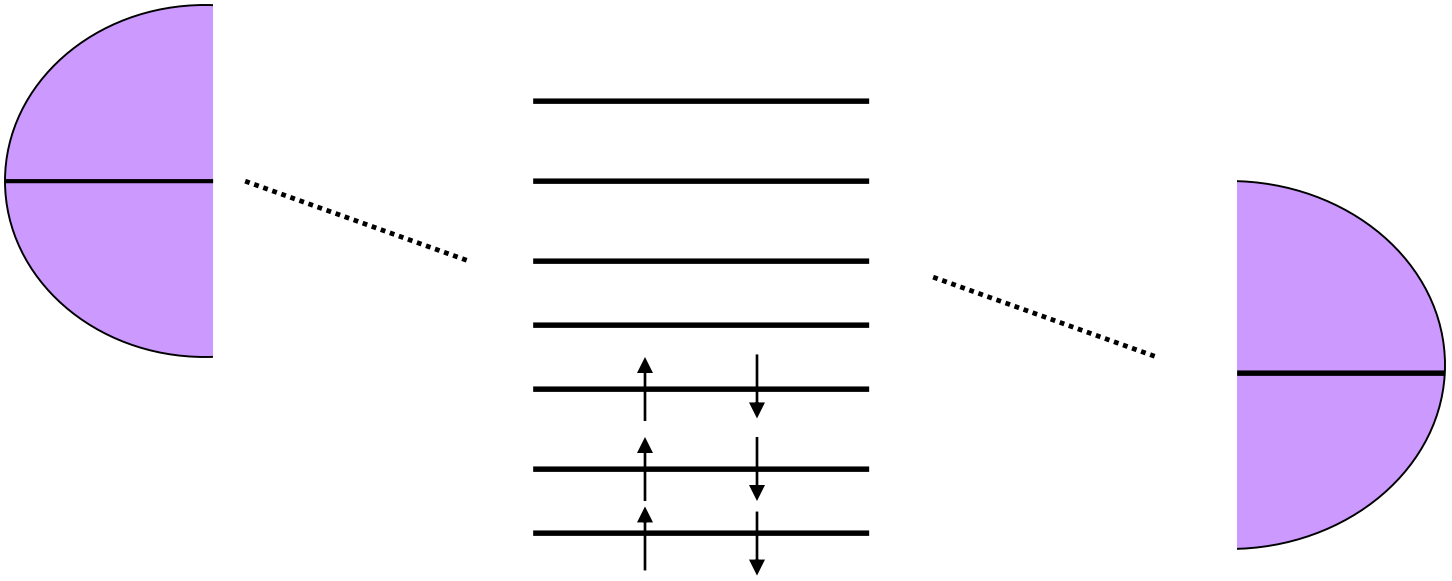




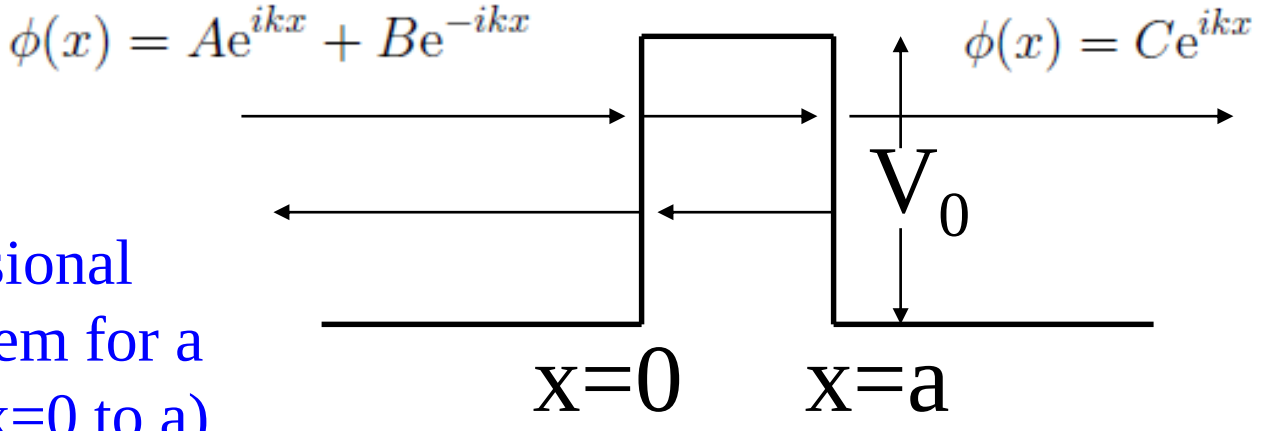
System connected to two reservoirs with different chemical potential



1. The left and right reservoirs are infinitely large and in thermo-equilibrium with different chemical potential.
2. They are connected via a small central region.
3. The total system may be in a non-equilibrium steady state that electrons flow steadily from the left to right.

One-dimensional scattering problem

The one-dimensional scattering problem for a potential wall (x=0 to a) can be solved analytically.



$V_0 < \varepsilon$

Reflection

$$\left|\frac{B}{A}\right|^2 = \left\{1 + \frac{4\varepsilon(\varepsilon - V_0)}{V_0^2 \sin^2(\kappa a)}\right\}^{-1}$$

Transmittance

$$\left|\frac{C}{A}\right|^2 = \left\{1 + \frac{V_0^2 \sin^2(\kappa a)}{4\varepsilon(\varepsilon - V_0)}\right\}^{-1}$$

$\varepsilon < V_0$ (Tunnel effect)

$$\left|\frac{C}{A}\right|^2 = \left\{1 + \frac{V_0^2 \sinh^2(\alpha a)}{4\varepsilon(V_0 - \varepsilon)}\right\}^{-1}$$

$$\varepsilon = \frac{\hbar^2}{2m}\kappa^2$$

Generalization of scattering problem in a quasi 1D

$$\begin{pmatrix} H_1 & \tau_1 & 0 \\ \tau_1^\dagger & H_d & t_2^\dagger \\ 0 & t_2 & H_2 \end{pmatrix} \begin{pmatrix} |\Psi_1\rangle \\ |\Psi_d\rangle \\ |\Psi_2\rangle \end{pmatrix} = E \begin{pmatrix} |\Psi_1\rangle \\ |\Psi_d\rangle \\ |\Psi_2\rangle \end{pmatrix}$$

(1) Assume that the wave function of the isolated lead is known.

$$H_1|\phi_{1,n}\rangle = E|\phi_{1,n}\rangle$$

(2) Assume that the whole wave function of the total system can be given by

$$\begin{pmatrix} |\Psi_1\rangle \\ |\Psi_d\rangle \\ |\Psi_2\rangle \end{pmatrix} = \begin{pmatrix} |\phi_{1,n}\rangle + |\chi_1\rangle \\ |\chi_d\rangle \\ |\chi_2\rangle \end{pmatrix}$$

(3) By putting the whole wave function in the step2 into the Schroedinger eq., we obtain the following equations:

$$|\psi_1\rangle = \left(1 + g_1\tau_1 G_d \tau_1^\dagger\right)|\phi_{1n}\rangle$$

$$|\psi_d\rangle = G_d\tau_1^\dagger|\phi_{1n}\rangle$$

$$|\psi_2\rangle = g_2\tau_2 G_d\tau_1^\dagger|\phi_{1n}\rangle$$

The whole wave function can be written by φ.

Charge density in the device

The charge density of the device can be calculated by considering the contribution produced with the incident wave function.

$$|\Psi_{d,n}^{(1)}\rangle = G_d \tau_1^\dagger \, |\phi_{1,n}\rangle$$

All the contributions are summed up with the Fermi function.

$$\begin{aligned}
\rho^{(1)} &= \int_{-\infty}^{\infty} dE \sum_n f(E,\mu_1)\delta(E-E_n)|\Psi_{d,n}^{(1)}\rangle\langle\Psi_{d,n}^{(1)}| \\
&= \int_{-\infty}^{\infty} dE f(E,\mu_1) \sum_n \delta(E-E_n) G_d\tau_1^\dagger|\phi_{1,n}\rangle\langle\phi_{1,n}|\tau_1 G_d^\dagger \\
&= \int_{-\infty}^{\infty} dE f(E,\mu_1) G_d\tau_1^\dagger \left(\sum_n \delta(E-E_n)|\phi_{1,n}\rangle\langle\phi_{1,n}|\right)\tau_1 G_d^\dagger \\
&= \int_{-\infty}^{\infty} dE f(E,\mu_1) G_d\tau_1^\dagger \frac{a_1}{2\pi}\tau_1 G_d^\dagger \qquad \Gamma_1 = \tau_1^\dagger a_1 \tau_1 \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} dE f(E,\mu_1) G_d \Gamma_1 G_d^\dagger
\end{aligned}$$

Adding the contributions from each lead yields

$$\rho = \frac{2}{2\pi}\sum_i \int_{-\infty}^{\infty} dE f\left(E,\mu_i\right) G_d \Gamma_i G_d^\dagger$$

Depending on the chemical potential, the contribution of each lead varies.

Flux of probability density #1

In the nonequilibrium steady state the probability density is conserved. We evaluate the flux of the probability density using the time-dependent Schroedinger equation.

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}|\Psi_1\rangle\\|\Psi_d\rangle\\|\Psi_2\rangle\end{pmatrix}=\begin{pmatrix}H_1 & \tau_1 & 0\\ \tau_1^\dagger & H_d & t_2^\dagger\\ 0 & t_2 & H_2\end{pmatrix}\begin{pmatrix}|\Psi_1\rangle\\|\Psi_d\rangle\\|\Psi_2\rangle\end{pmatrix}$$

The time evolution of the integrated probability density is given by

$$\begin{aligned}\frac{\partial}{\partial t}\langle\Psi_d|\Psi_d\rangle &= \frac{\partial\langle\Psi_d|}{\partial t}|\Psi_d\rangle+\langle\Psi_d|\frac{\partial|\Psi_d\rangle}{\partial t}\\ &= \frac{i}{\hbar}\left[\left(\langle\Psi_2|\tau_2+\langle\Psi_d|H_d+\langle\Psi_1|\tau_1\right)|\Psi_d\rangle\right.\\ &\quad\left.-\langle\Psi_d|\left(\tau_1^\dagger|\Psi_1\rangle+H_d|\Psi_d\rangle+\tau_2^\dagger|\Psi_2\rangle\right)\right]\\ &= \frac{i}{\hbar}\left[\left(\langle\Psi_1|\tau_1|\Psi_d\rangle-\langle\Psi_d|\tau_1^\dagger|\Psi_1\rangle\right)+\left(\langle\Psi_2|\tau_2|\Psi_d\rangle-\langle\Psi_d|\tau_2^\dagger|\Psi_2\rangle\right)\right]\end{aligned}$$

Each term can be regarded as the contribution from each lead k.

$$i_k=-\frac{ie}{\hbar}\left(\langle\psi_k|\tau_k|\psi_d\rangle-\langle\psi_d|\tau_k^\dagger|\psi_k\rangle\right)$$

Thus, we have $\sum_k i_k = 0$

Flux of probability density #2

$$i_k = -\frac{ie}{\hbar}\left(\langle\psi_k|\tau_k|\psi_d\rangle - \langle\psi_d|\tau_k^\dagger|\psi_k\rangle\right)$$

where the sign of the flux of the probability density i_k is taken so that the direction from the device to the lead k can be positive.

i_1 Flux from the device to the lead 1 ←

i_2 Flux from the device to the lead 2 →

In other words, in the steady state i_1 from the device to the lead 1 is equal to $-i_2$ from the lead 2 to the device.

$$i_1 = -i_2$$

Current #1

Ψ_d and Ψ_2 can be written by the wave function of the isolated lead 1.

$$\left|\psi_d\right\rangle = G_d \tau_1^\dagger \left|\phi_{1n}\right\rangle \qquad \left|\psi_2\right\rangle = g_2 \tau_2 G_d \tau_1^\dagger \left|\phi_{1n}\right\rangle$$

Then, the current from the leads 1 to 2 is given by

$$\begin{aligned} i_{1\to 2} &= -\frac{ie}{\hbar}\left(\left\langle\psi_2\right|\tau_2\left|\psi_d\right\rangle - \left\langle\psi_d\right|\tau_2^\dagger\left|\psi_2\right\rangle\right) \\ &= -\frac{ie}{\hbar}\left(\left\langle\phi_{1n}\right|\tau_1 G_d^\dagger \tau_2^\dagger g_2^\dagger \tau_2 G_d \tau_1^\dagger\left|\phi_{1n}\right\rangle - \left\langle\phi_{1n}\right|\tau_1 G_d^\dagger \tau_2^\dagger g_2 \tau_2 G_d \tau_1^\dagger\left|\phi_{1n}\right\rangle\right) \\ &= -\frac{ie}{\hbar}\left\langle\phi_{1n}\right|\tau_1 G_d^\dagger \tau_2^\dagger \left(g_2^\dagger - g_2\right)\tau_2 G_d \tau_1^\dagger\left|\phi_{1n}\right\rangle \\ &= \frac{e}{\hbar}\left\langle\phi_{1n}\right|\tau_1 G_d^\dagger \Gamma_2 G_d \tau_1^\dagger\left|\phi_{1n}\right\rangle \end{aligned}$$

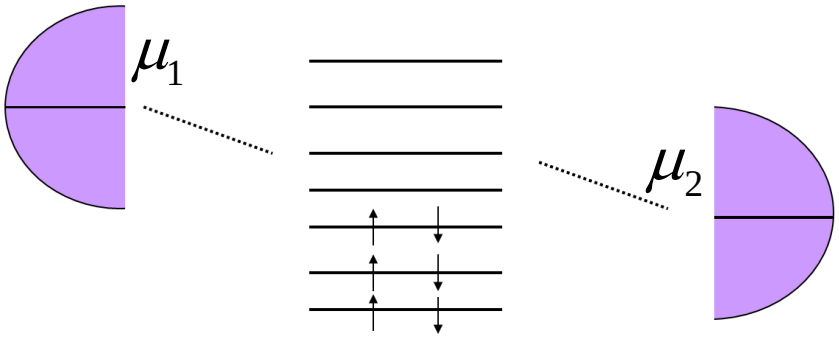
Current #2

Considering all the states in the lead 1, we obtain the formula of current from the leads 1 to 2 as follows:

$$I_{1\to 2} = 2\frac{e}{\hbar}\int_{-\infty}^{\infty} dE\, f\left(E,\mu_1\right)\sum_n \delta\left(E-E_n\right)\left\langle \phi_{1n}\left|\tau_1 G_d^{\dagger}\Gamma_2 G_d \tau_1^{\dagger}\right|\phi_{1n}\right\rangle$$

$$= \frac{2e}{h}\int_{-\infty}^{\infty} dE\, f\left(E,\mu_1\right)\mathrm{Tr}\left(G_d^{\dagger}\Gamma_2 G_d \Gamma_2\right)$$

Adding all the contributions from each lead yields the formula:



$$I = \frac{2e}{h}\int_{-\infty}^{\infty} dE\left(f\left(E,\mu_1\right) - f\left(E,\mu_2\right)\right)\mathrm{Tr}\left(G_d^{\dagger}\Gamma_2 G_d \Gamma_2\right)$$

Transmission

Summary of the formulae

The whole wave function is written by the incident wave function:

$$|\psi_1\rangle = \left(1 + g_1 \tau_1 G_d \tau_1^\dagger\right)|\phi_{1n}\rangle$$

$$|\psi_d\rangle = G_d \tau_1^\dagger |\phi_{1n}\rangle$$

$$|\psi_2\rangle = g_2 \tau_2 G_d \tau_1^\dagger |\phi_{1n}\rangle$$

The charge density in the device is given by the sum of the contributions from each lead.

$$\rho = \frac{2}{2\pi} \sum_i \int_{-\infty}^{\infty} dE f\left(E, \mu_i\right) G_d \Gamma_i G_d^\dagger$$

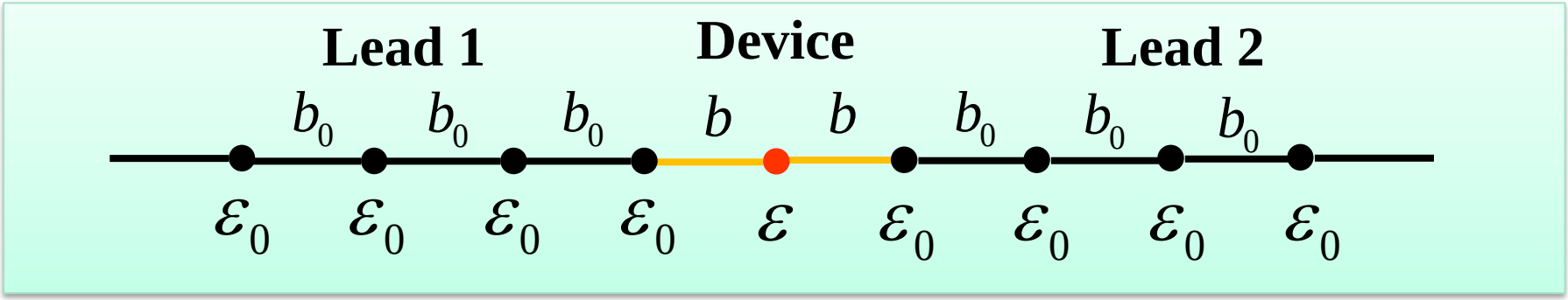
Considering the flux of the probability density, the current is given by

$$I = \frac{2e}{h} \int_{-\infty}^{\infty} dE \left(f\left(E, \mu_1\right) - f\left(E, \mu_2\right)\right) \mathrm{Tr}\left(G_d^\dagger \Gamma_2 G_d \Gamma_2\right)$$

Transmission

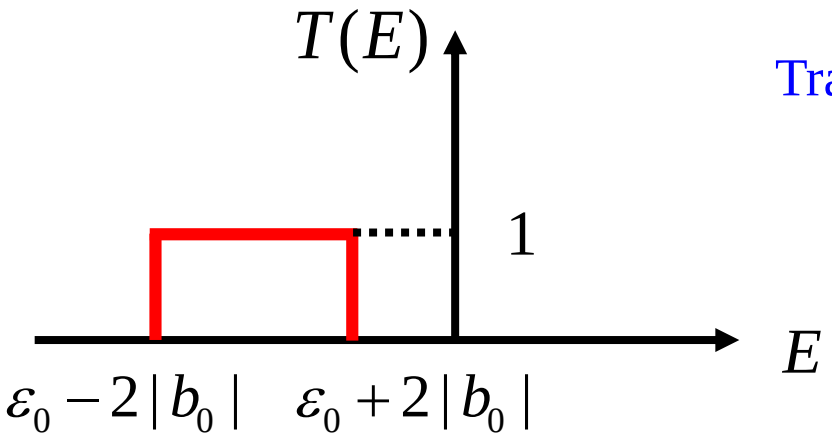
Linear chain model

As a simple case, Let's consider a linear chain mode as shown below:



Surface Green functions: $$g_1(Z) = g_2(Z) = \frac{Z - \varepsilon_0 - \sqrt{(Z-\varepsilon_0)^2 - 4b_0^2}}{2b_0^2}$$

Self-energies: $$\Sigma_1(Z) = \Sigma_2(Z) = \frac{b^2}{2b_0^2}\left(Z - \varepsilon_0 - \sqrt{(Z-\varepsilon_0)^2 - 4b_0^2}\right)$$



Transmission:

$$T(E) = \mathrm{Tr}(G_d^{\dagger}\Gamma_2 G_d \Gamma_1) = 1$$

$$\varepsilon_0 - 2|b_0| < E < \varepsilon_0 + 2|b_0|$$

$$T(E) = 0 \quad \text{Otherwise}$$

Conductance and transmission

Starting from the Landauer formula:

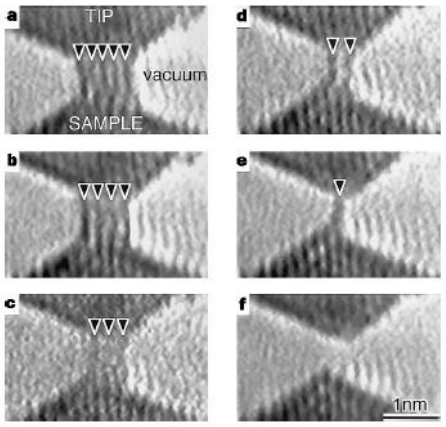
$$I = \frac{2e}{h}\int_{-\infty}^{\infty} dE\left(f\left(E,\mu_1\right) - f\left(E,\mu_2\right)\right)\mathrm{T}\left(E\right)$$

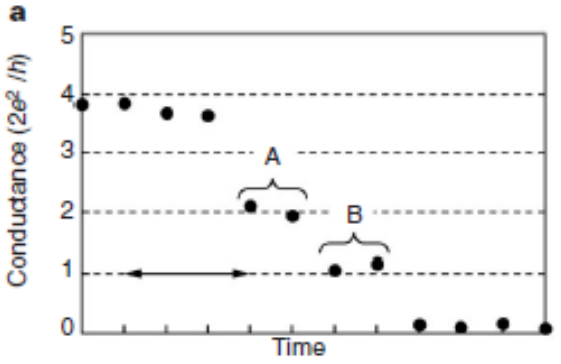
one can obtain the following formula at a small V.

$$I \simeq V\left(T\left(\mu\right)\frac{2e^2}{h}\right) \qquad G = T\left(\mu\right)G_0$$

Conductance quantum:

$$G_0 = \frac{2e^2}{h}$$

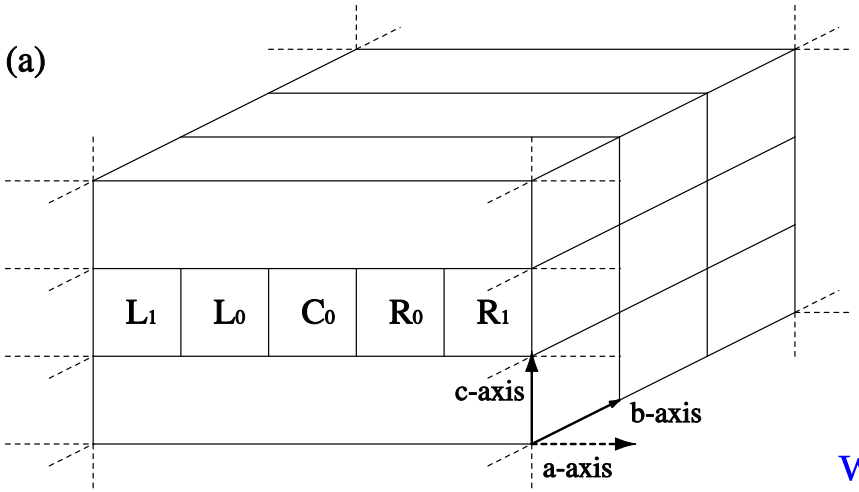


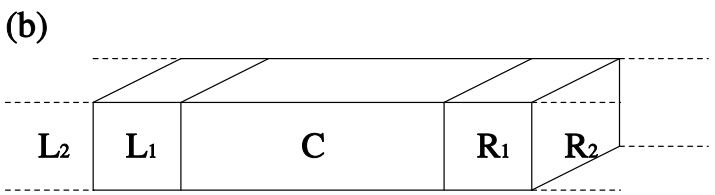


Takayanagi et al.,
Nature **395**, 780 (1998).

3D cases

Assume that the periodicity on the bc plane, and non-periodicity along the a-axis.





TO et al., PRB 81, 035116 (2010).

Then, we can write the Bloch wave function on the bc plane

$$\psi^{(\mathbf{k})}_{\sigma\nu}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathrm{n}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}_{\mathrm{n}}} \sum_{i\alpha} c^{(\mathbf{k})}_{\sigma\nu,i\alpha} \phi_{i\alpha}(\mathbf{r} - \tau_i - \mathbf{R}_{\mathrm{n}}),$$

and the problem can be cast to a 1D problem

$$H^{(\mathbf{k})}_{\sigma} c^{(\mathbf{k})}_{\sigma\nu} = \varepsilon^{(\mathbf{k})}_{\sigma\nu} S^{(\mathbf{k})} c^{(\mathbf{k})}_{\sigma\nu},$$

where the Hamiltonian is given by a block tri-diagonal form:

$$H^{(\mathbf{k})}_{\sigma} = \begin{pmatrix} \ddots & \ddots & & & 0 \\ \ddots & H^{(\mathbf{k})}_{\sigma,L_1} & H^{(\mathbf{k})}_{\sigma,L_1C} & & \\ & H^{(\mathbf{k})}_{\sigma,CL_1} & H^{(\mathbf{k})}_{\sigma,C} & H^{(\mathbf{k})}_{\sigma,CR_1} & \\ & & H^{(\mathbf{k})}_{\sigma,R_1C} & H^{(\mathbf{k})}_{\sigma,R_1} & \ddots \\ 0 & & & \ddots & \ddots \end{pmatrix}$$

Green function of the device region

Using the block form of matrices and the following identity:

$$G_{\sigma}^{(\mathbf{k})}(Z)(ZS^{(\mathbf{k})} - H_{\sigma}^{(\mathbf{k})}) = \mathrm{I}$$

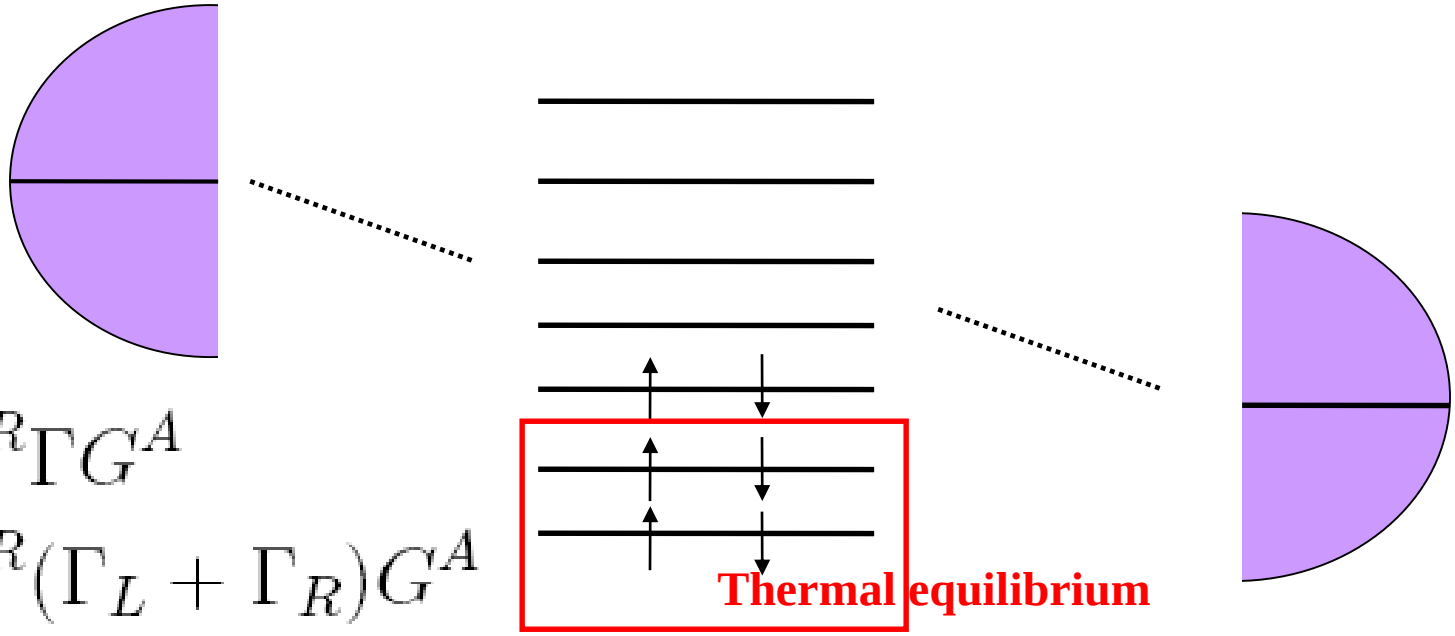
we obtain

$$G_{\sigma,C}^{(\mathbf{k})}(Z) = \left(ZS_{C}^{(\mathbf{k})} - H_{\sigma,C}^{(\mathbf{k})} - \Sigma_{\sigma,L}^{(\mathbf{k})}(Z) - \Sigma_{\sigma,R}^{(\mathbf{k})}(Z)\right)^{-1}$$

where the self energies are explicitly given by

$$\begin{aligned}
\Sigma_{\sigma,L}^{(\mathbf{k})}(Z) &= (ZS_{CL_1}^{(\mathbf{k})} - H_{\sigma,CL_1}^{(\mathbf{k})}) \times \\
&\quad G_{\sigma,L}^{(\mathbf{k})}(Z)(ZS_{L_1C}^{(\mathbf{k})} - H_{\sigma,L_1C}^{(\mathbf{k})}), \\
\Sigma_{\sigma,R}^{(\mathbf{k})}(Z) &= (ZS_{CR_1}^{(\mathbf{k})} - H_{\sigma,CR_1}^{(\mathbf{k})}) \times \\
&\quad G_{\sigma,R}^{(\mathbf{k})}(Z)(ZS_{R_1C}^{(\mathbf{k})} - H_{\sigma,R_1C}^{(\mathbf{k})}),
\end{aligned}$$

Assumption in the implementation of the NEGF method



$$G^{<} = G^{R}\Gamma G^{A}$$
$$= G^{R}(\Gamma_L + \Gamma_R)G^{A}$$

It is assumed that the states for $\mu_R < \mu_L$ in the central part is in the thermal equilibrium. Then, the charge density can be calculated by

$$\rho = -\frac{2}{\pi}\mathrm{Im}\int dE f_R G^R - \frac{2}{\pi}\mathrm{Im}\int dE (f_L - f_R) G^R \Gamma_L G^A$$

Density matrix of the device region

From the previous assumption we made, the density matrix is given by the sum of the equilibrium and nonequilibrium contributions.

$$\rho^{(\mathrm{neq})}_{\sigma,\mathbf{R}_\mathrm{n}} = \rho^{(\mathrm{eq})}_{\sigma,\mathbf{R}_\mathrm{n}} + \Delta\rho_{\sigma,\mathbf{R}_\mathrm{n}}.$$

The equilibrium contribution is given by the integration of the equilibrium Green function.

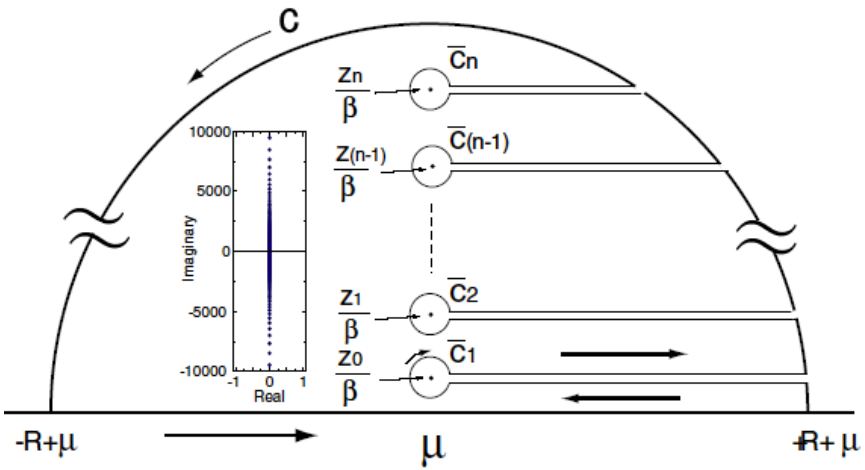
$$\rho^{(\mathrm{eq})}_{\sigma,\mathbf{R}_\mathrm{n}} = \frac{1}{V_\mathrm{c}} \int_{\mathrm{BZ}} dk^3 \left(\rho^{(\mathbf{k})}_{\sigma,+} - \rho^{(\mathbf{k})}_{\sigma,-} \right) \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{R}_\mathrm{n}}$$

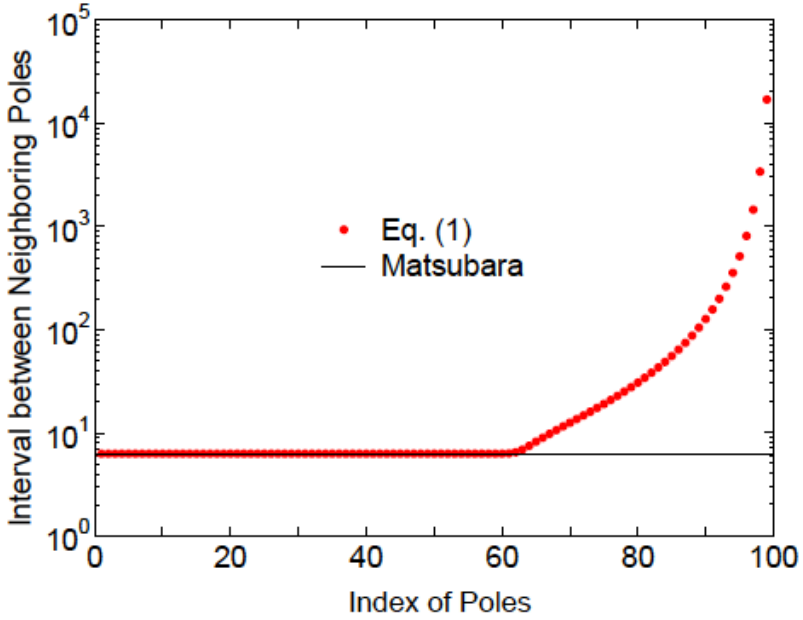
$$\rho^{(\mathbf{k})}_{\sigma,\pm} = \frac{i}{2\pi} \int_{-\infty}^{\infty} dE G^{(\mathbf{k})}_{\sigma,C}(E \pm i0^+) f(E-\mu),$$

Contour integration

$$\frac{1}{1+\exp(x)} = \frac{1}{2} - \frac{x}{4}\left(\cfrac{1}{1+\cfrac{(\frac{x}{2})^2}{3+\cfrac{(\frac{x}{2})^2}{5+\cfrac{(\frac{x}{2})^2}{\cdots \over (2M-1)+\ddots}}}}\right)$$

By expressing the Fermi function one can obtain a special distribution of poles. The distribution gives the extremely fast convergence.





T. Ozaki, PRB 75, 035123 (2007).

Nonequlibrium density matrix

Since NEGF is a non-analytic function, the integration is performed on the real axis with a small imaginary part.

$$\Delta\rho_{\sigma,\mathbf{R}_\mathrm{n}} = \frac{1}{V_\mathrm{c}} \int_\mathrm{BZ} dk^3 \Delta\rho_\sigma^{(\mathbf{k})} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{R}_\mathrm{n}}$$

$$\begin{aligned}\Delta\rho_\sigma^{(\mathbf{k})} &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dE G_{\sigma,C}^{(\mathbf{k})}(E+i\epsilon)\Gamma_{\sigma,\mathrm{s}_1}^{(\mathbf{k})}(E) \\ &\qquad \times G_{\sigma,C}^{(\mathbf{k})}(E-i\epsilon)\Delta f(E)\end{aligned}$$

$$\Gamma_{\sigma,\mathrm{s}_1}^{(\mathbf{k})}(E) = i\left(\Sigma_{\sigma,\mathrm{s}_1}^{(\mathbf{k})}(E+i\epsilon) - \Sigma_{\sigma,\mathrm{s}_1}^{(\mathbf{k})}(E-i\epsilon)\right)$$

$$\Delta f(E) = f(E-\mu_{\mathrm{s}_1}) - f(E-\mu_{\mathrm{s}_2}).$$

Poisson eq. with the boundary condition

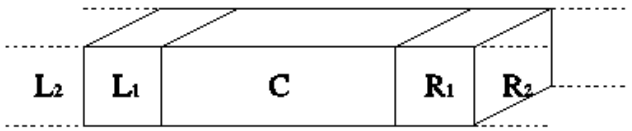
Poisson eq.

$$\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right)V_{\mathrm{H}}(x,y,z)=-4\pi\rho(x,y,z)$$

FT for x-y plane

$$\left(\frac{d^2}{dz^2}-G_{\parallel}\right)V_{\mathrm{H}}(G_{\parallel},z)=-4\pi\rho(G_{\parallel},z)$$

Discretization



$$\frac{V_{\mathrm{H}}(G_{\parallel},z_{n+1})-2V_{\mathrm{H}}(G_{\parallel},z_n)V_{\mathrm{H}}(G_{\parallel},z_{n-})}{(\Delta z)^2}-\rho(G_{\parallel},z)V_{\mathrm{H}}(G_{\parallel},z_n)=-4\pi\rho(G_{\parallel},z_n)$$

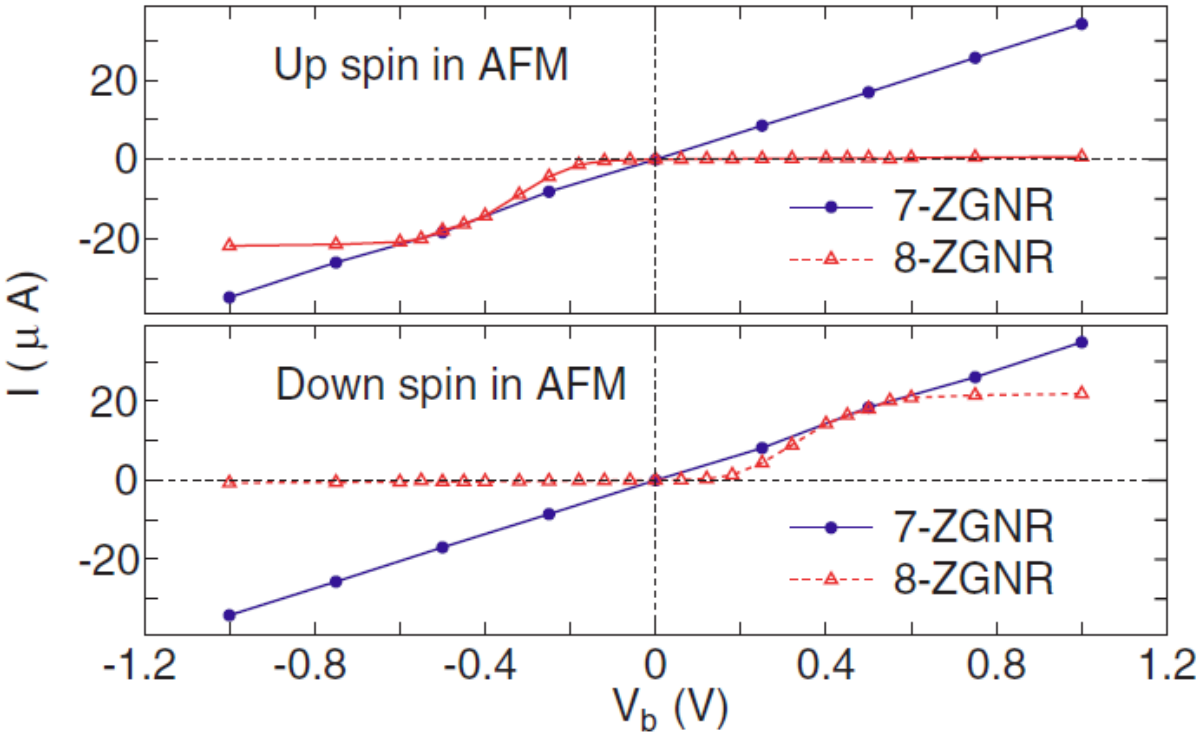
Boundary conditions: $V_{\mathrm{H}}(G_{\parallel},z_0)$ $V_{\mathrm{H}}(G_{\parallel},z_N)$

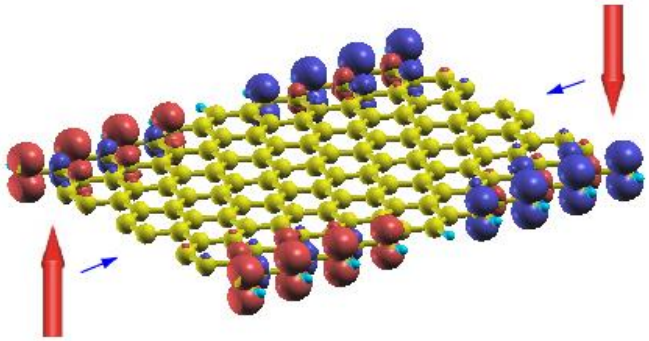
XY-FFT → linear eq. → XY-inverse FFT

Cost: $O(N_x\log(N_x))\times O(N_y\log(N_y))\times O(N_z)$

Dual spin filter effect of the magnetic junction

Rectification ratio at 0.4V: 44.3





PRB 81, 075422 (2010).

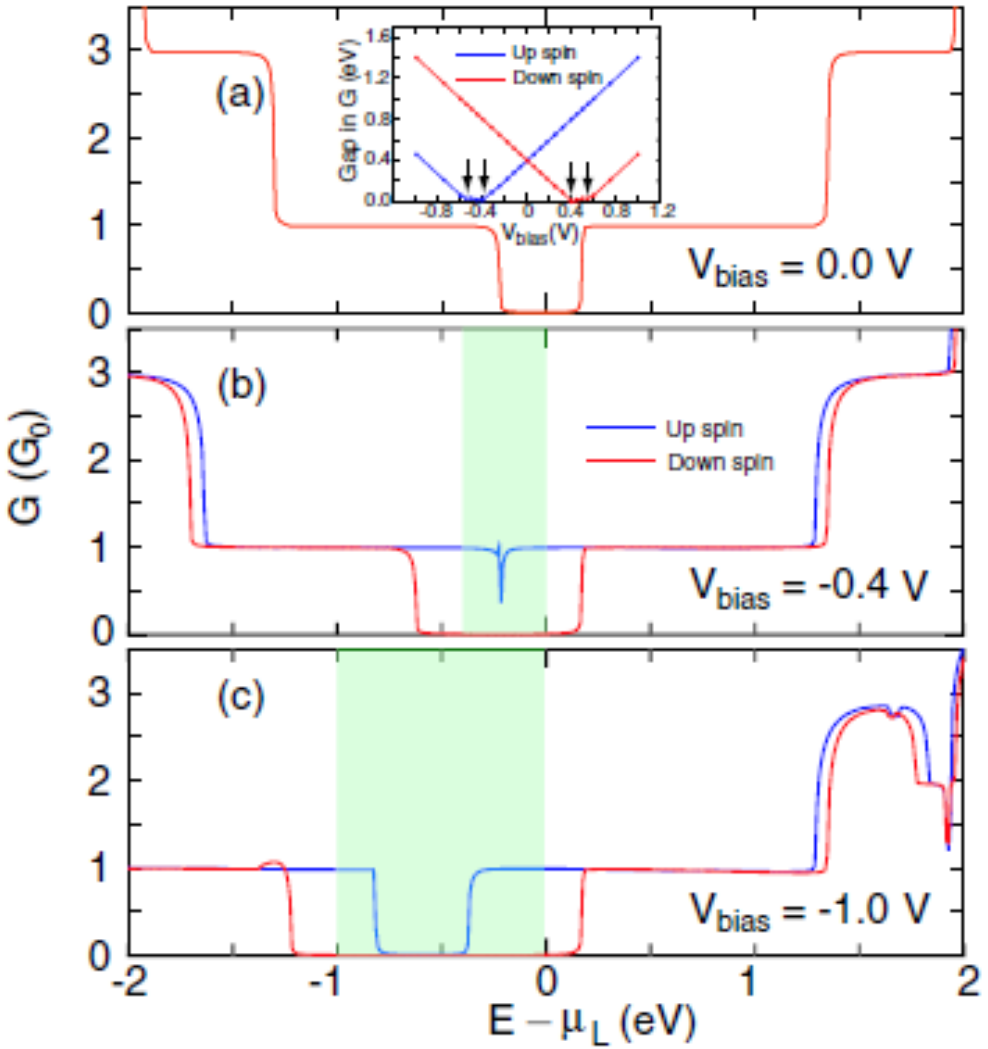
up spin : flowing from left to right

down spin: flowing from right to left

→ Dual spin filter effect

The same result is obtained for 6-ZGNR and 10-ZGNR.

Conductance (transmission) of 8-ZGNR



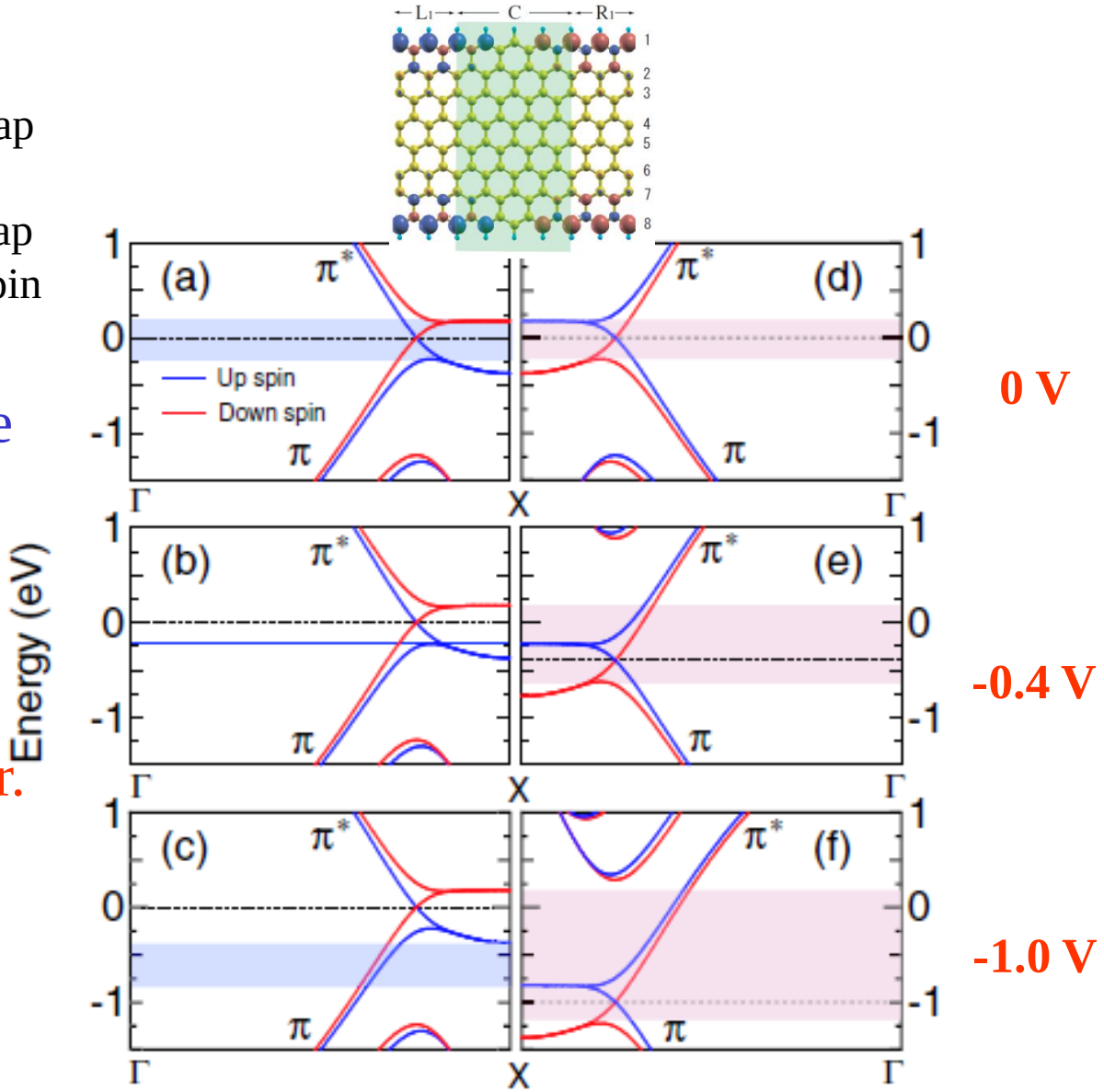
For the up-spin channel, the conduction gap disappears at -0.4 V, while the gap keep increasing for the down spin channel.

Band structures with offset of 8-ZGNR

Blue shade: Conductance gap for the up spin

Purple shade: Conductance gap for the down spin

The energy regime where the conductance gap appears does correspond to the energy region where only the π and π* states overlaps each other.



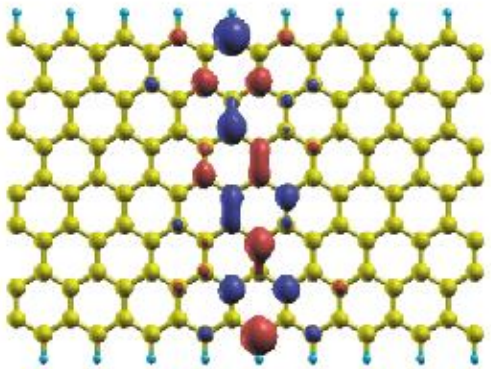
Wannier functions of π and π* states

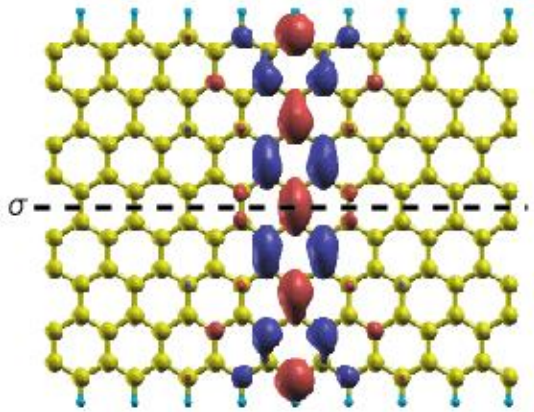
calculated from by Marzari's method

7-ZGNR

8-ZGNR

π^*

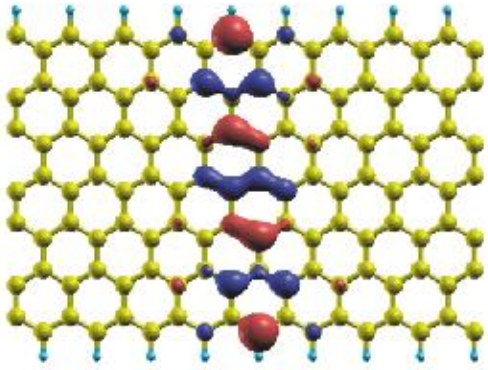


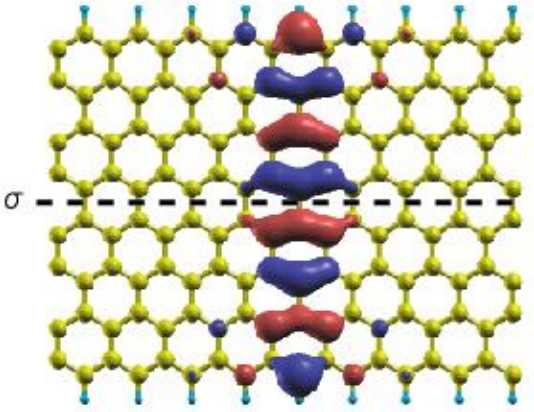


Symmetric

Neither symmetric nor asymmetric

π

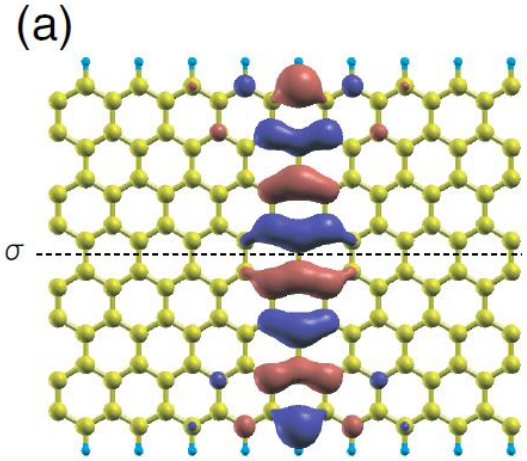




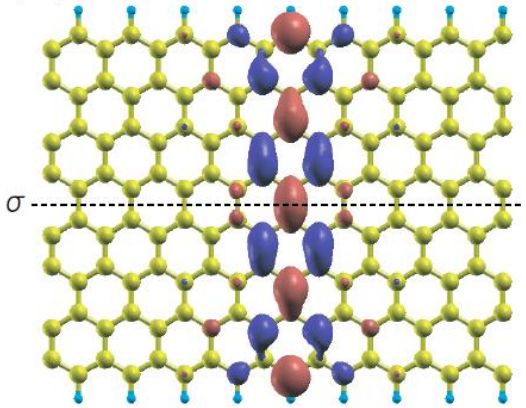
Asymmetric

Wannier functions for π and π* states of 8-ZGNR

Wannier function of π



Wannier function of π *



Since for 8-ZGNR the π state is asymmetric and the π* state is symmetric with respect to the σ mirror plane, the hopping integrals are zero.

Hopping integrals calculated by the Wannier functions

TABLE I: Tight-binding parameters (eV) evaluated by WFs denoted by WF, and a fitting, denoted by *fitted*, for the π and π^* states of the non-spin polarized 8-ZGNR, where ε is the on-site energy, and h_1, $h_2 \cdots$ the nearest and the second nearest neighbor hopping integrals, and so on. The Fermi level is set to zero.

	ε	h_1	h_2	h_3	h_4
π (WF)	-1.3609	-0.7660	0.0076	0.0529	-0.0352
π^* (WF)	1.4486	0.7708	-0.0400	-0.0513	0.0269
π (fitted)	-1.4165	-0.7083	0	0	0
π^* (fitted)	1.4135	0.7067	0	0	0

Since the π and π* states of 7-ZGNR are neither symmetric nor asymmetric, the corresponding hopping integrals survive.

I-V curve by a TB model

In the simplified TB model the current can be written by

$$I = \int dE(f_L - f_R)T(E),$$

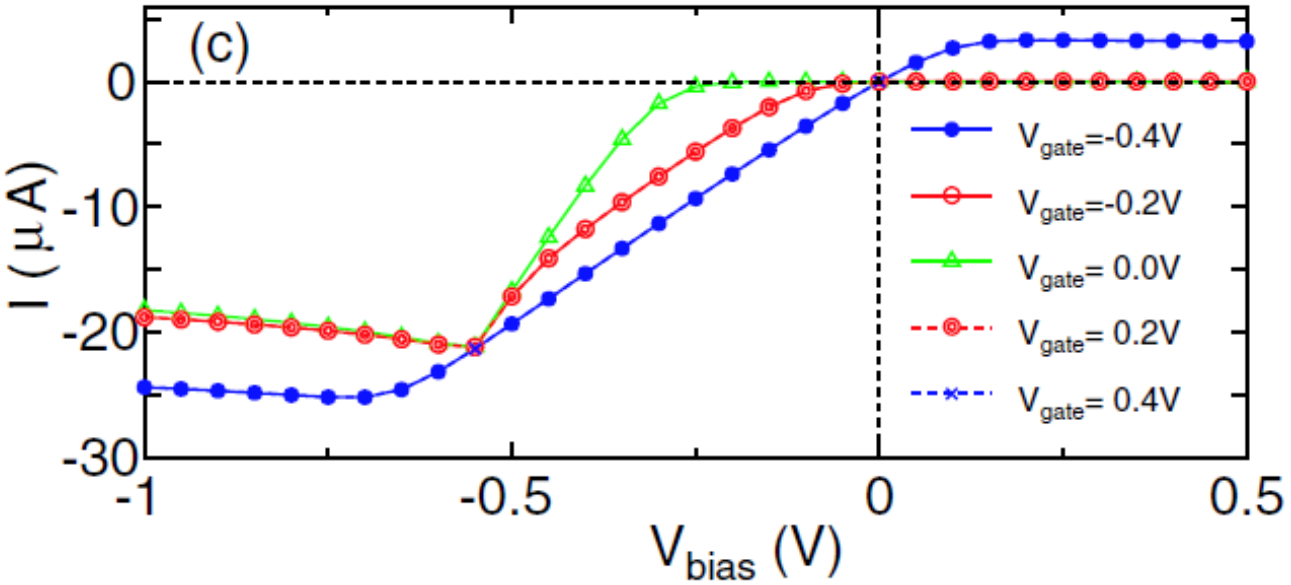
$$T(E) = \frac{4S_L(E)S_R(E)}{[S_L(E) + S_R(E)]^2}$$

$$S_L(E) = \sqrt{4h_1^2 - \left[E - (\varepsilon - \frac{1}{2}\Delta_x)\right]^2},$$

$$S_R(E) = \sqrt{4h_1^2 - \left[E - (\varepsilon + \frac{1}{2}\Delta_x + V_{\text{bias}})\right]^2},$$

I-V by the simplified TB model

The TB model well reproduces the result of the NEGF calculation.



Computational flow

The calculation proceeds as step 1 → step 2 → step 3.

1. Band calculations

The band structure calculations are performed for the left and right leads using a program code 'openmx'. The calculated results will be used to represent the Hamiltonian of the leads in the NEGF calculation of the step 2.

2. NEGF calculation

The NEGF calculation is performed for the structure of L0|C0|R0 under zero or a finite bias voltage using a program code 'openmx', where the result in the step 1 is used for the construction of the leads.

3. Transmission and current

By making use of the result of the step 2, the transmission, charge/spin current density, and the eigenchannel are calculated by a program code 'openmx'.

All the details can be found at the pages 161-183 in the manual.

Exercises

- Calculate the transmission of carbon chain. Please follow the guidance in the pages 162-172 of the manual. The input files, ‘Lead-Chain.dat’ and ‘NEGF-Chain.dat’, are available in the directory ‘work/negf_example’.

- Calculate the transmission of graphene. The input files, ‘Lead-Graphene.dat’ and ‘NEGF-Graphene.dat’, are available in the directory ‘work/negf_example’.

Exercise 1: carbon chain

Step 1

% ./openmx Lead-Chain.dat

Output: lead-chain.hks

Step 2 & 3

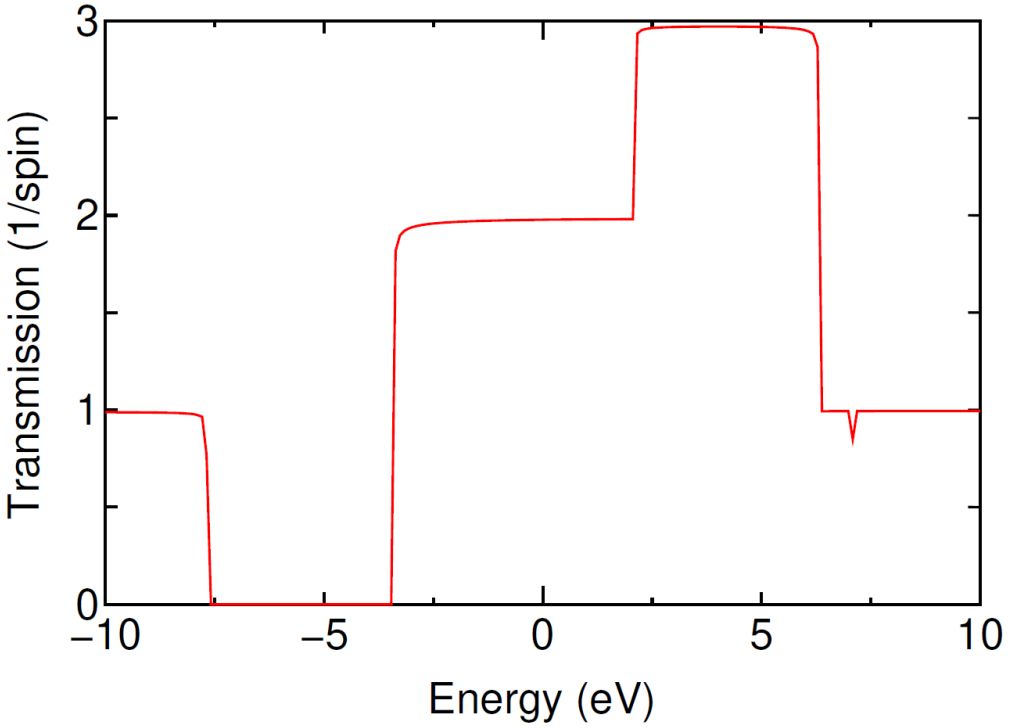
% ./openmx NEGF-Chain.d

Output:
negf-chain.tran0_0
negf-chain.conductance
…

The input files can be found i
work/negf_example/

Step 1: Lead-Chain.dat
Step 2&3: NEGF-Chain.dat

You can get the following transmission by plotting negf-chain.tran0_0, where x: 4th column, y: 6th column.



Exercise 2: Graphene

Step 1

% ./openmx Lead-Graphene.dat

Output: lead-graphene.hks

Step 2 & 3

% ./openmx NEGF-Graphene.dat

Output:
negf-graphene.tran0_0
negf-graphene.tran1_0
…….

The input files can be found in

work/negf_example/

Step 1: Lead-Graphene.dat
Step 2&3: NEGF-Graphene.dat

You can get the following transmission by plotting gra-negf.tran5_0, where x: 4th column, y: 6th column.