First-principles electronic transport calculations

- Electronic transport in nano-scale materials:
- Experiments
- Nonequilibrium Green function method
  - From a scattering problem
  - Keldysh method
- Applications

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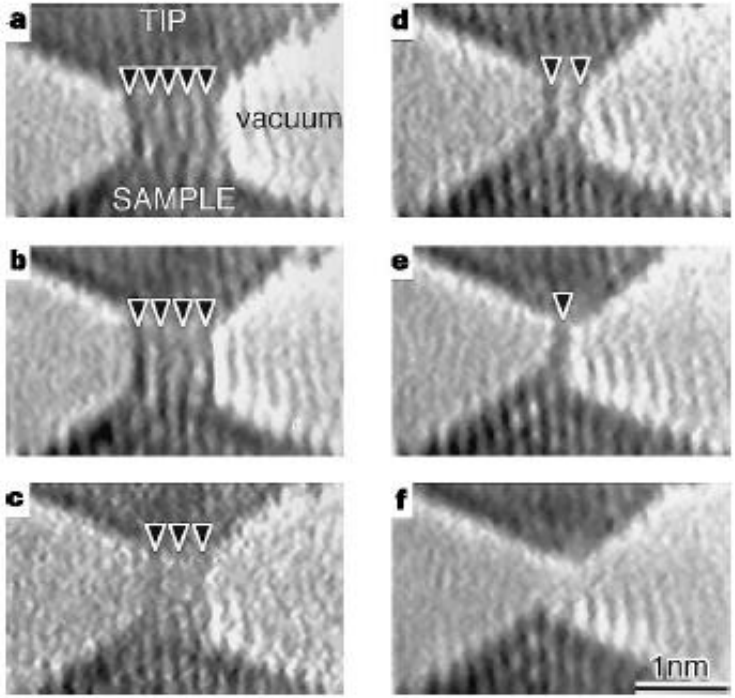
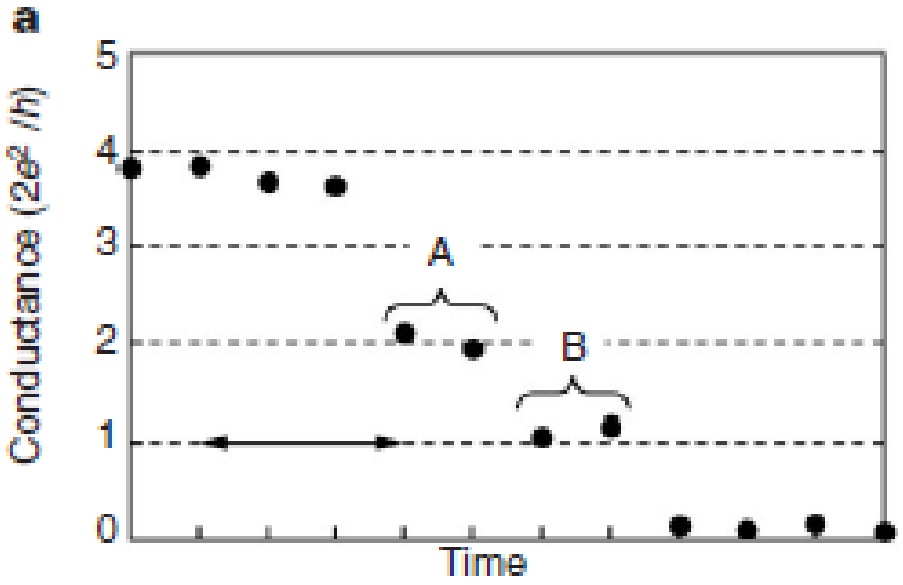
Quantum conductance in gold nanowires

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.

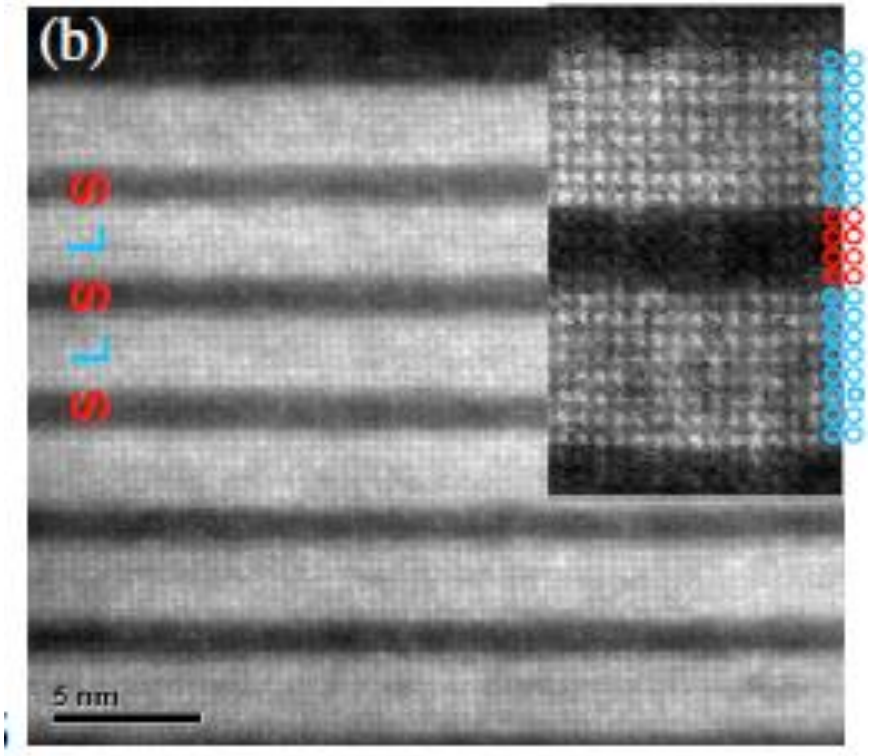


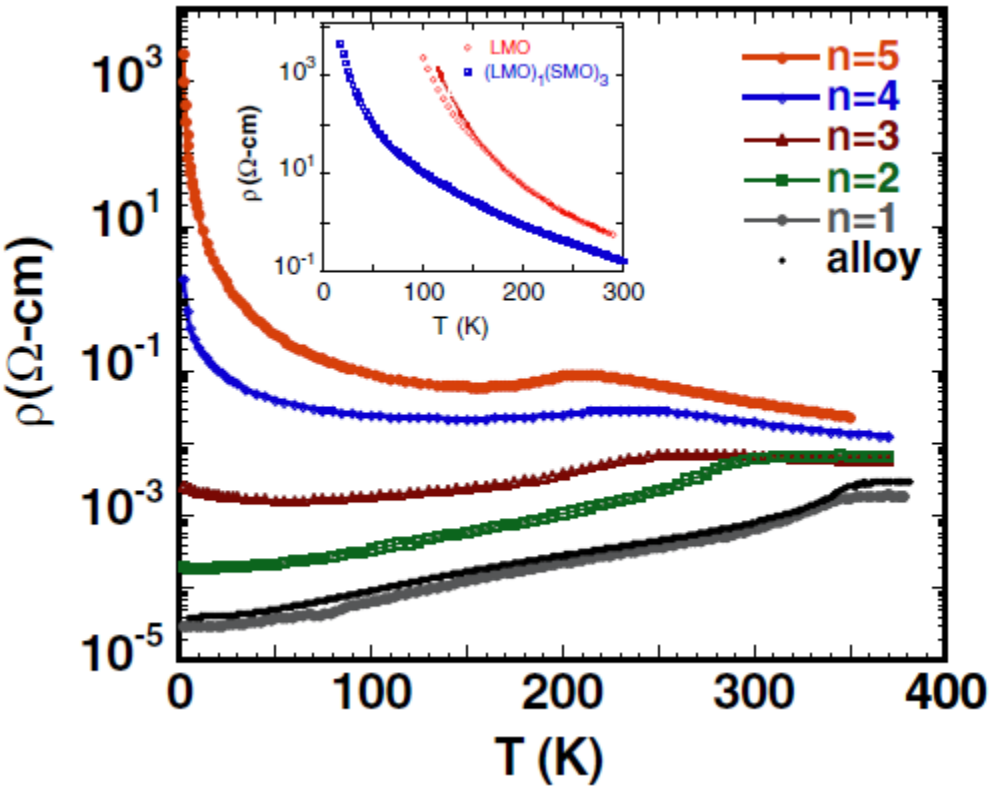


Takayanagi et al., Nature **395**, 780 (1998).

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

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

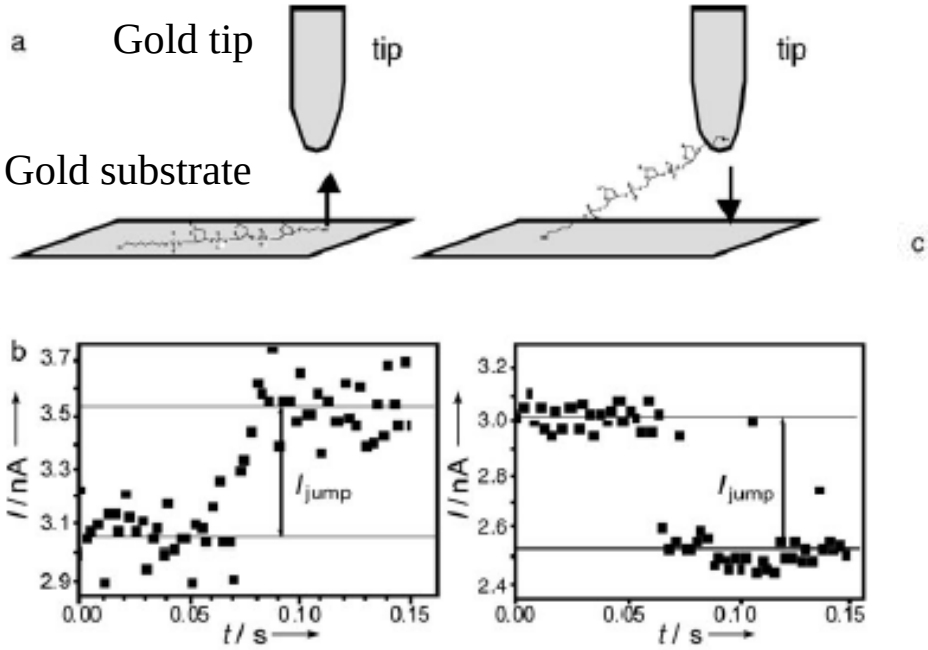




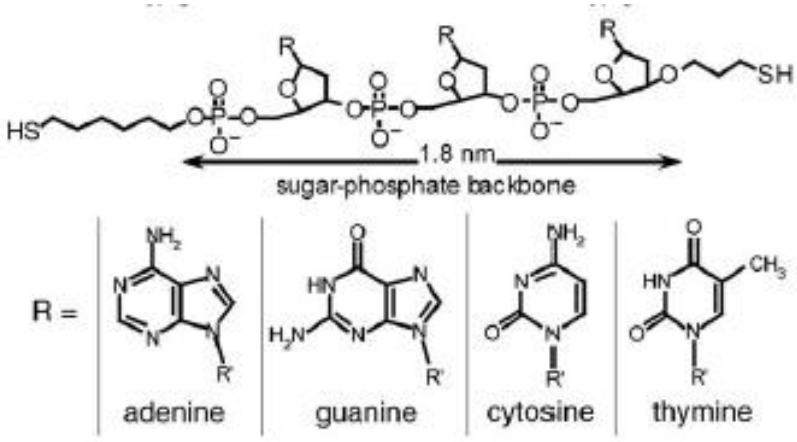
Bhattacharya et al., PRL **100,** 257203 (2008)

Transport in a single strand DNA molecule

Adsorption Detachment



Molecular structure of a single strand DNA molecule

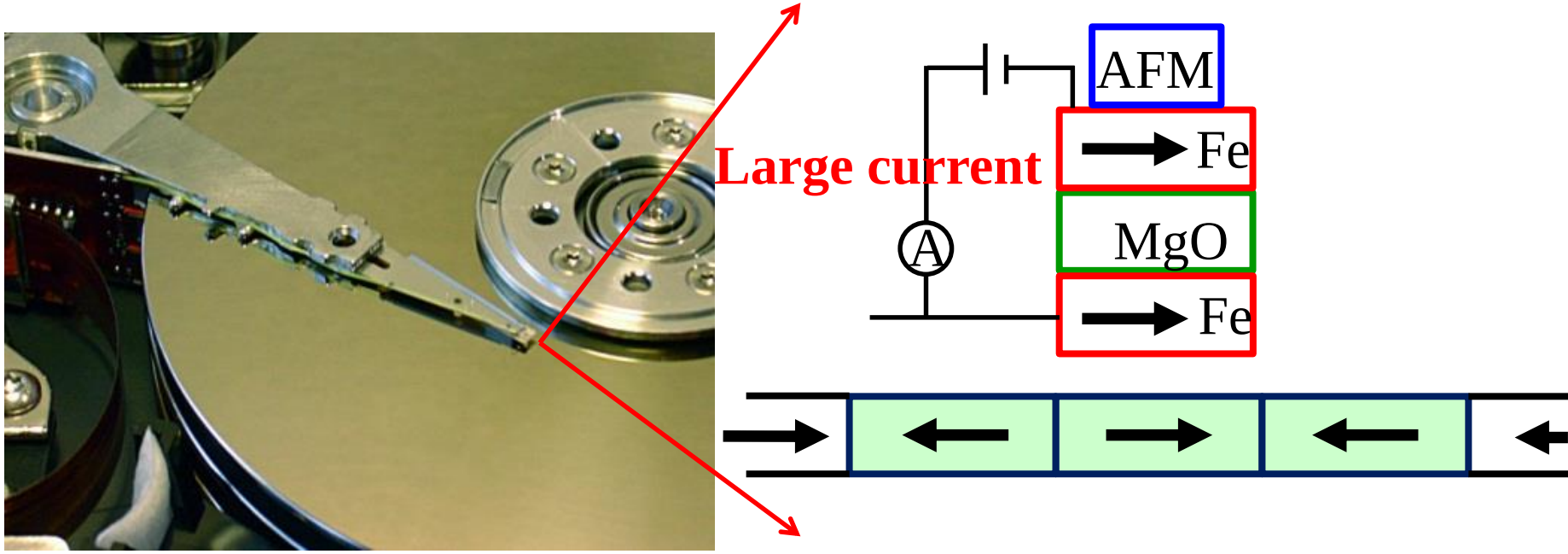


The current jumps when the molecule adsorbs and detaches.

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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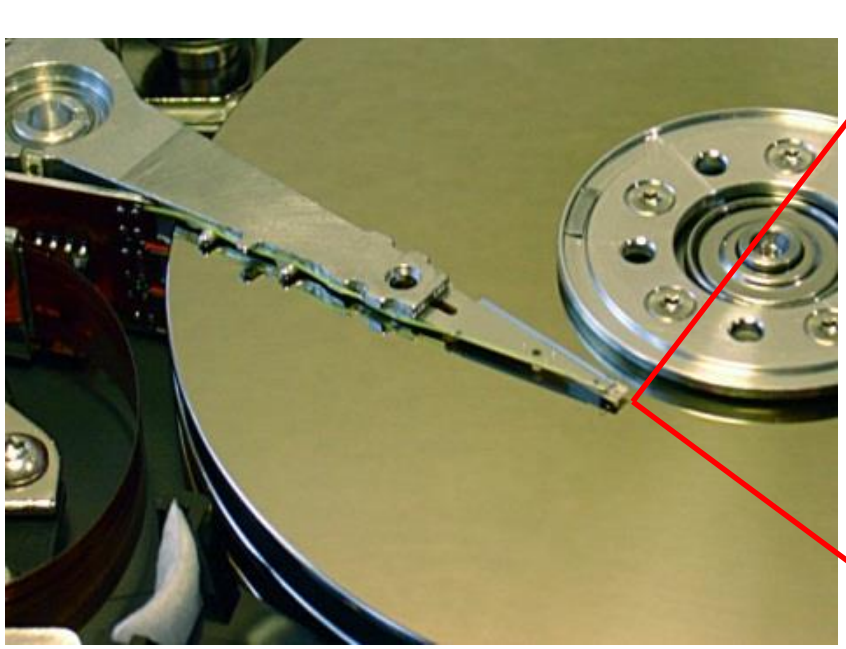
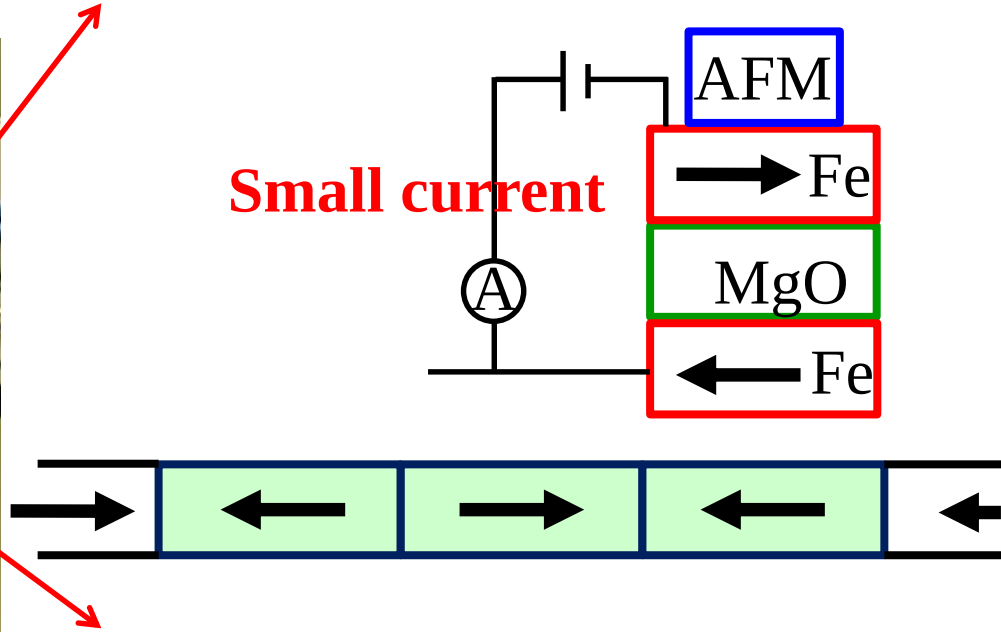




Nonequilibrium Green funtion methods

1961 Schwinger

Perturbation theory for $-\infty$ to $t=\infty$

1965 Keldysh

Keldysh Green function method

1972 Caroli et al.,

Application of the Keldysh Green function method

2002 Brandbyge et al.,

Development of Transiesta (ATK)

Potential advantages of the NEGF method

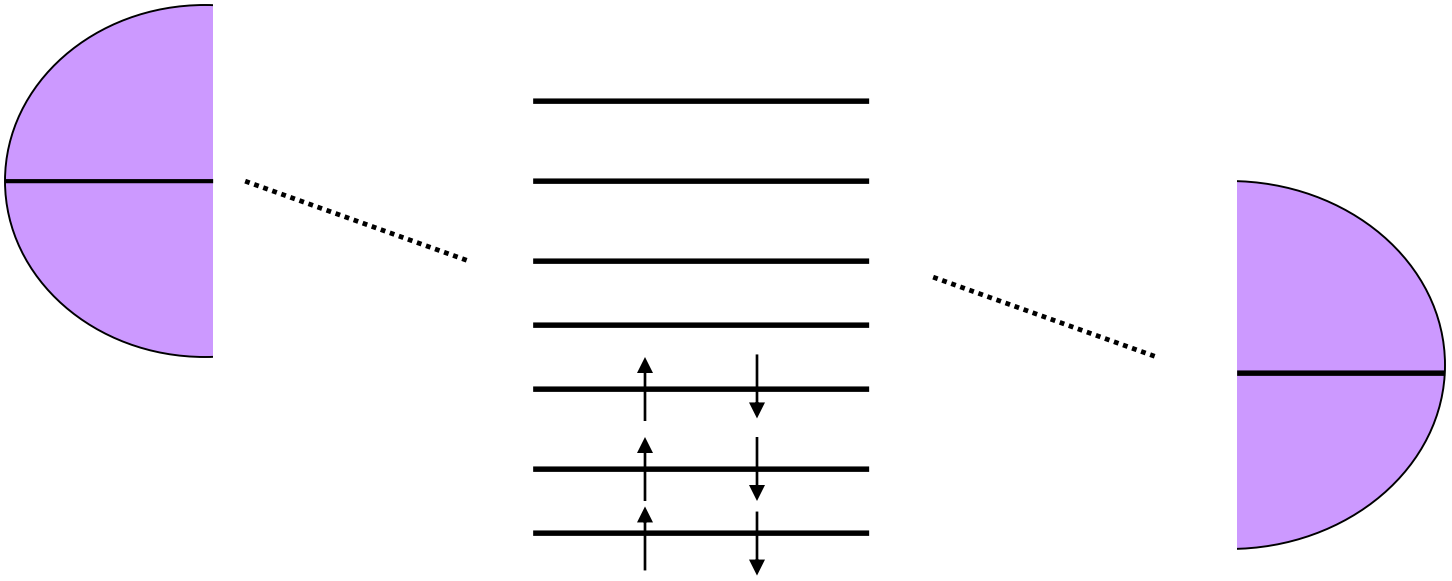
1. The source and drain contacts are treated based on the same theoretical framework as for the scattering region.
2. The electronic structure of the scattering region under a finite source-drain bias voltage is self-consistently determined by combining with first principle electronic structure calculation methods such as the density functional theory (DFT) and the Hartree-Fock (HF) method.
3. Many body effects in the transport properties, e.g., electron-phonon
4. Its applicability to large-scale systems can be anticipated, since the NEGF method relies practically on the locality of basis functions in real space, resulting in computations for sparse matrices.

Derivation of the NEGF method

1. From a scattering problem
2. From Keldysh Green funtion

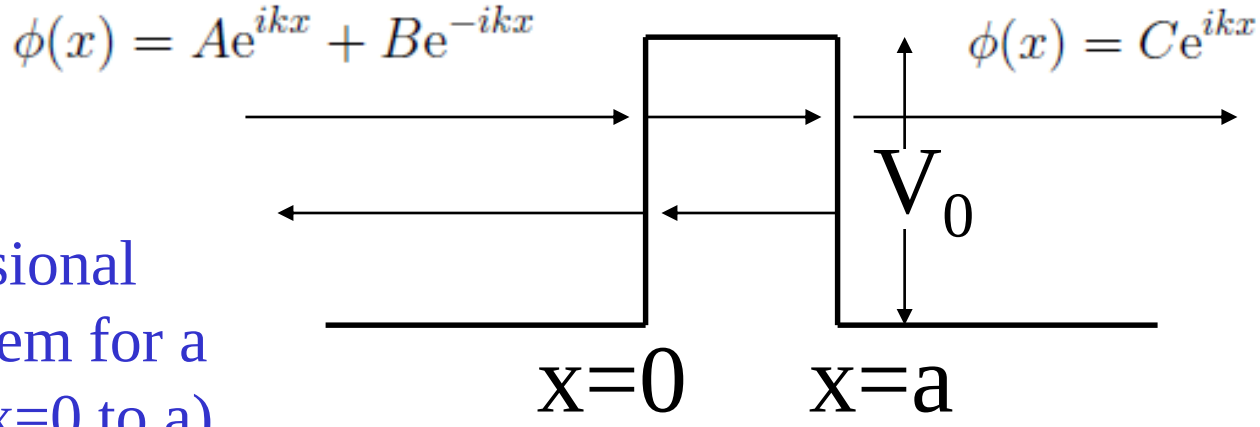
Within one-particle picture, both the methods give the same framework.

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:

$$|\Psi_1\rangle = (1 + g_1\tau_1 G_d \tau_1^\dagger)\ |\phi_{1,n}\rangle$$

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

$$|\Psi_2\rangle = g_2\tau_2 G_d \tau_1^\dagger |\phi_{1,n}\rangle$$

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.

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

Adding the contributions from each lead yields

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

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

Flux of probability density (1)

In the nonequilibrium steady state, assuming that the probability density conserves, and 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 the lead k to the device can be positive.

i_1 Flux from the lead 1 to the device →

i_2 Flux from the lead 2 to the device ←

In other words, in the steady state the flux (i_1) of the probability density from the lead 1 to the device is equal to that ($-i_2$) from the device to the lead 2. Note that the sign of i_2 is opposite to that of i_1 when they are seen as current.

Current (1)

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

$$|\Psi_d\rangle = G_d\tau_1^\dagger\ |\phi_{1,n}\rangle \qquad |\Psi_2\rangle = g_2\tau_2 G_d\tau_1^\dagger|\phi_{1,n}\rangle$$

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

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

Current (2)

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

$$
\begin{aligned}
I_{2 \text{ from } 1} &= 2\frac{e}{\hbar}\int_{E=-\infty}^{\infty} \mathrm{d}E\, f(E,\mu_1)\sum_n \delta(E-E_n)\langle\psi_{1,n}|\tau_1 G_d^\dagger \Gamma_2 G_d \tau_1^\dagger|\psi_{1,n}\rangle \\
&= \frac{2e}{\hbar}\int_{E=-\infty}^{\infty} \mathrm{d}E\, f(E,\mu_1)\sum_{m,n} \delta(E-E_n)\langle\psi_{1,n}|\tau_1|m\rangle\langle m|G_d^\dagger \Gamma_2 G_d \tau_1^\dagger|\psi_{1,n}\rangle \\
&= \frac{2e}{\hbar}\int_{E=-\infty}^{\infty} f(E,\mu_1)\sum_m \langle m|G_d^\dagger \Gamma_2 G_d \tau_1^\dagger \left(\sum_n \delta(E-E_n)|\psi_{1,n}\rangle\langle\psi_{1,n}|\right)\tau_1|m\rangle \\
&= \frac{2e}{\hbar}\int_{E=-\infty}^{\infty} \mathrm{d}E\, f(E,\mu_1)\sum_m \langle m|G_d^\dagger \Gamma_2 G_d \tau_1^\dagger \frac{a_1}{2\pi}\tau_1|m\rangle \\
&= \frac{e}{\pi\hbar}\int_{E=-\infty}^{\infty} \mathrm{d}E\, f(E,\mu_1)\mathrm{Tr}\left(G_d^\dagger \Gamma_2 G_d \Gamma_1\right)
\end{aligned}
$$

Adding all the contributions from each lead yields the formula:

$$
I = \frac{e}{\pi\hbar}\int_{E=-\infty}^{\infty} \mathrm{d}E\, (f(E,\mu_1)-f(E,\mu_2))\,\mathrm{Tr}\left(G_d^\dagger \Gamma_2 G_d \Gamma_1\right)
$$

← Transmission

Summary: from a scattering problem

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

$$|\Psi_1\rangle = (1 + g_1\tau_1 G_d \tau_1^\dagger)\ |\phi_{1,n}\rangle$$

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

$$|\Psi_2\rangle = g_2\tau_2 G_d\tau_1^\dagger |\phi_{1,n}\rangle$$

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

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

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

$$I = \frac{e}{\pi\hbar}\int_{E=-\infty}^{\infty} \mathrm{d}E\,(f(E,\mu_1) - f(E,\mu_2))\,\mathrm{Tr}\left(G_d^\dagger \Gamma_2 G_d \Gamma_1\right)$$

Transmission

Conductance and transmission

Let us start an expression of current I

$$I = \frac{q}{h} \int dE\, T(E) \left[f(E - \mu_1) - f(E - \mu_2) \right], \tag{1}$$

where q is the elementary charge, h the Plank constant, T the transmission, f the Fermi function, μ_1 and μ_2 the chemical potentials of the left and right leads.

Our purpose is to find a relation:

$$I = \frac{V}{R} = VG, \tag{2}$$

where V is the source-drain bias voltage, R the resistance, and $G \equiv \frac{1}{R}$ is the conductance. To derive Eq. (2) based on Eq. (1), we consider a case that $\mu_1 = \mu_2 + qV = \mu + qV$ with a tiny V. Then, Eq. (1) can be approximated by

$$\begin{aligned} I &= \frac{q}{h} \int dE\, T(E) \left[f(E - (\mu + qV)) - f(E - \mu) \right], \\ &\simeq \int dE \left(T(\mu) + \frac{\partial T(E)}{\partial E}|_{E=\mu} (E - \mu) \right) \left[f(E - (\mu + qV)) - f(E - \mu) \right] \\ &\quad + \int dE\, T(E) \left[f(E - \mu) + \frac{\partial f(E - (\mu + qV))}{\partial V}|_{V=0} V - f(E - \mu) \right]. \end{aligned} \tag{3}$$

Conductance and transmission: continued

Since the first term in the R.H.S of Eq. (3) is zero when $V \to 0$, and $\frac{\partial f(E-(\mu+qV))}{\partial V}|_{V=0} = -q\frac{\partial f(E-(\mu+qV))}{\partial E}|_{V=0}$, we obtain

$$I \simeq \frac{q^2}{h} V \int dE\, T(E) \left(-\frac{\partial f(E-(\mu+qV))}{\partial E}|_{V=0} \right). \quad (4)$$

In case that $V \to 0$ and the elecronic temperature is zero, the derivative in Eq. (4) becomes the delta function. Thus, we have

$$I \simeq V \left(T(\mu)\frac{q^2}{h} \right). \quad (5)$$

By comparing Eqs. (2) and (5), the conductance G can be related to the transmission at the chemical potential:

$$G = T(\mu)\frac{q^2}{h}. \quad (6)$$

Here we define

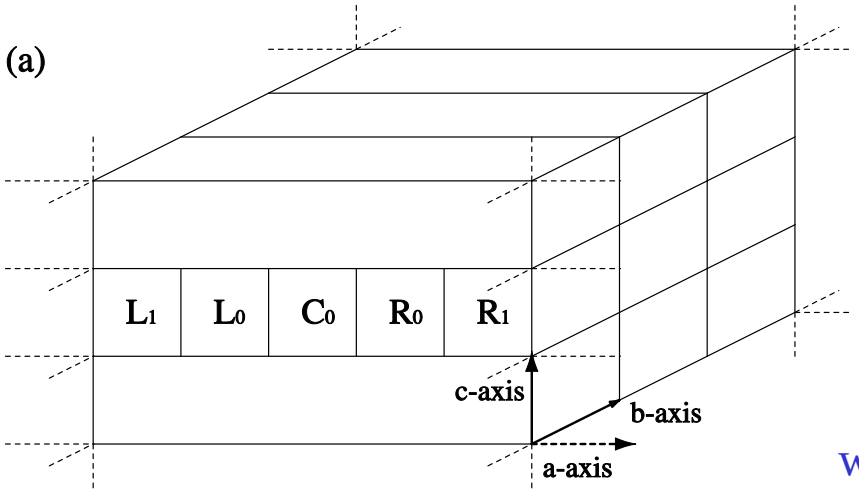
$$G_0 = \frac{q^2}{h}. \quad (7)$$

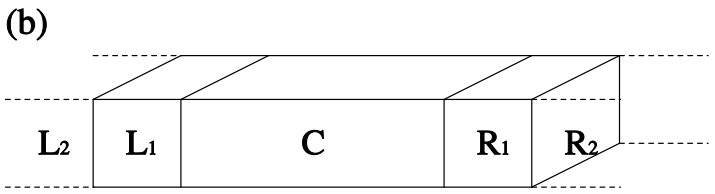
Using G_0 as unit, we can write

$$G = T(\mu) \qquad \text{in } G_0 \quad (8)$$

System we consider

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





T. Ozaki et al., PRB 81, 035116 (2010).

Thus, 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:

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

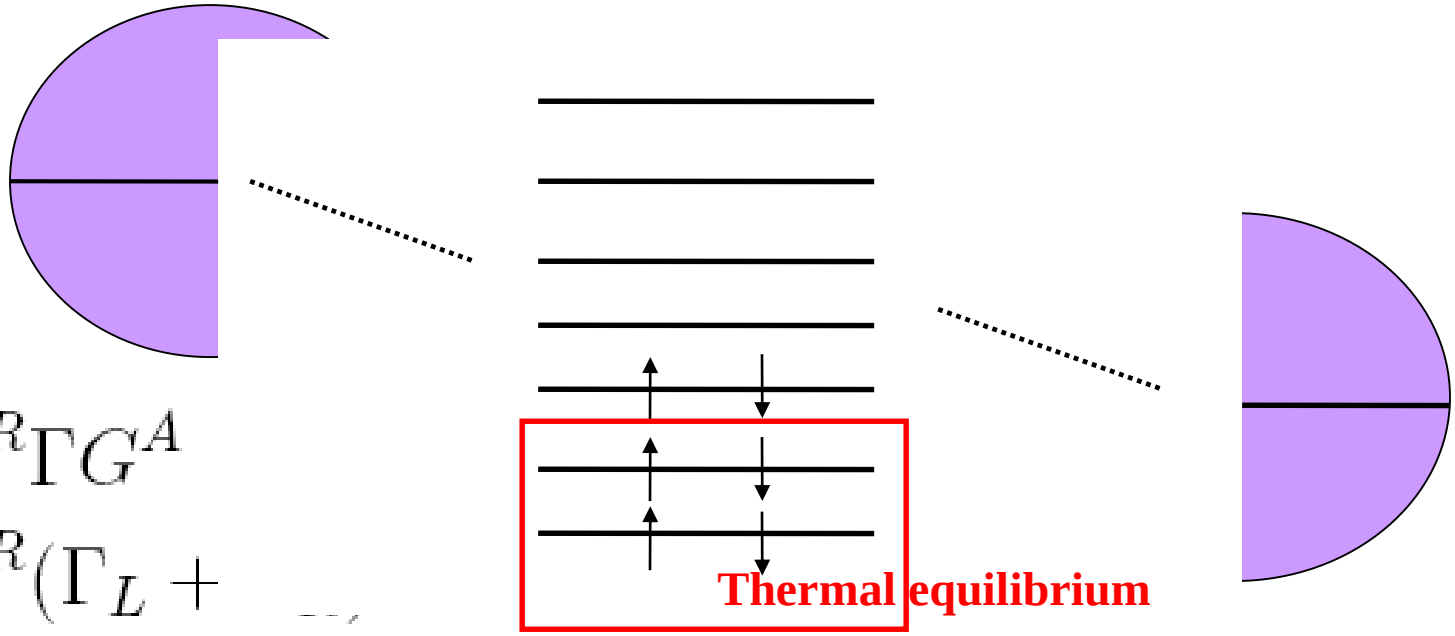
we obtain

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

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



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

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.

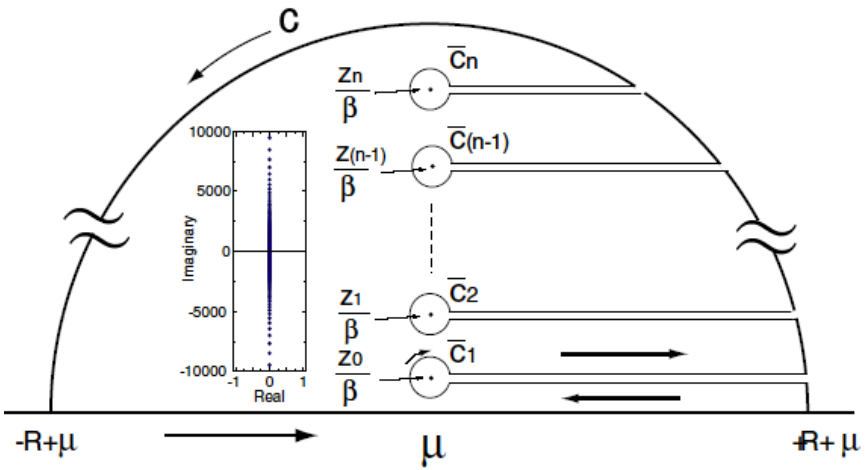
$$\rho^{(\mathrm{eq})}_{\sigma,\mathbf{R}_\mathrm{n}} = \frac{1}{V_\mathrm{c}} \int_{\mathrm{BZ}} dk^3 \left(\rho^{(\mathbf{k})}_{\sigma,+} - \rho^{(\mathbf{k})}_{\sigma,-} \right) \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{R}_\mathrm{n}}$$

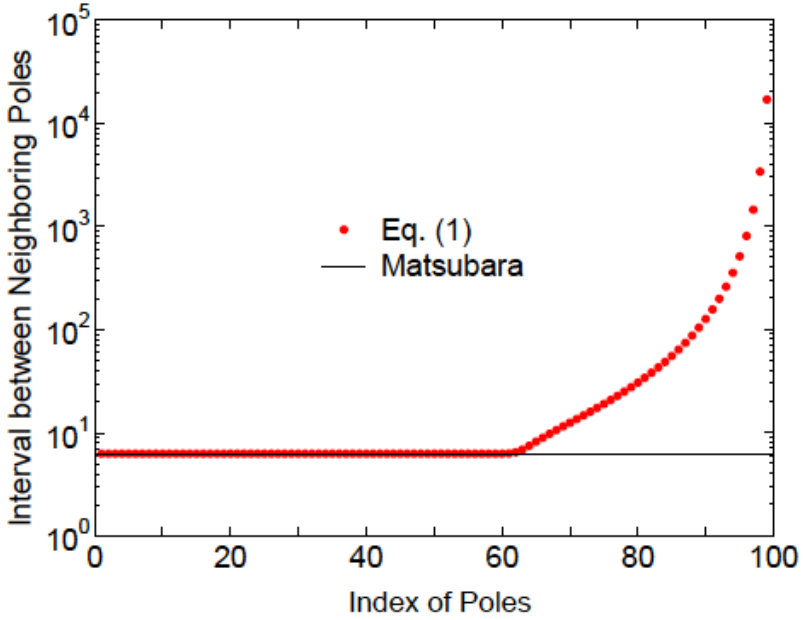
$$\rho^{(\mathbf{k})}_{\sigma,\pm} = \frac{i}{2\pi} \int_{-\infty}^{\infty} dE G^{(\mathbf{k})}_{\sigma,C}(E \pm i0^+) f(E-\mu),$$

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

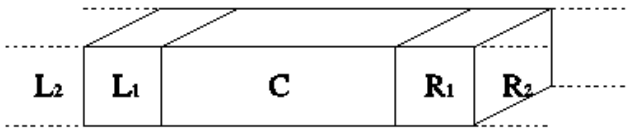
Poisson eq.

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

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



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

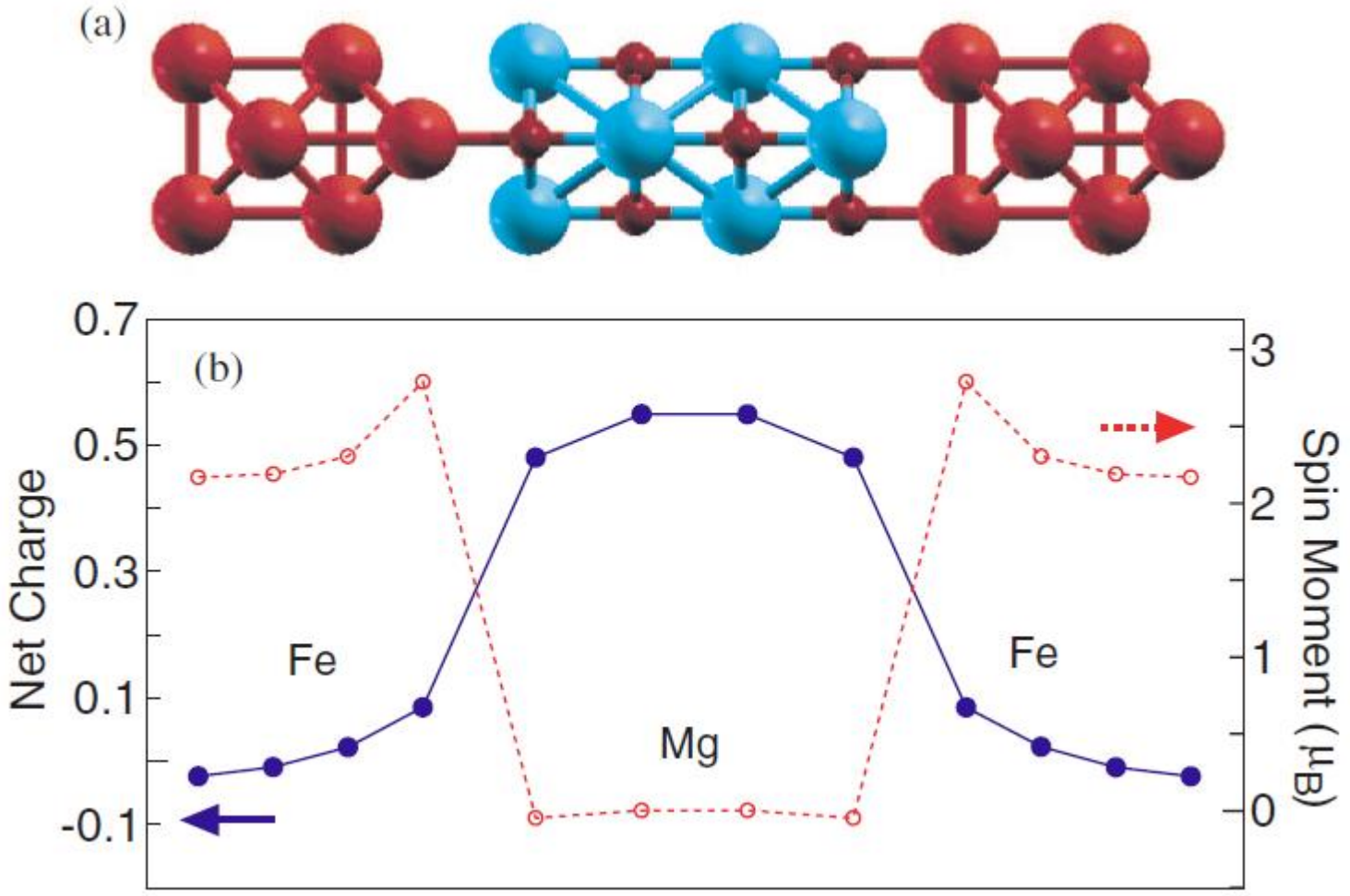
Boundary conditions: $V_{\mathrm{H}}(G_{\parallel},z_0)$ $V_{\mathrm{H}}(G_{\parallel},z_N)$

XY-FFT → linear eq. → XY-inverse FFT

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

Fe|MgO|Fe (TMR device)

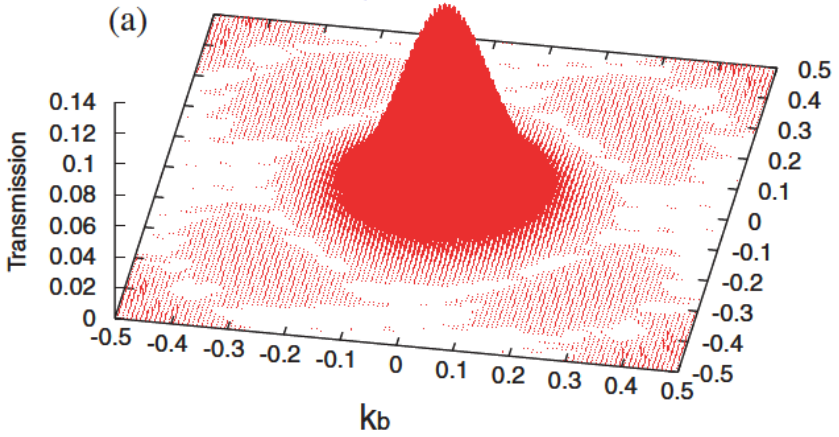
Fe|MgO|Fe device has been gradually used as a hard disk head.



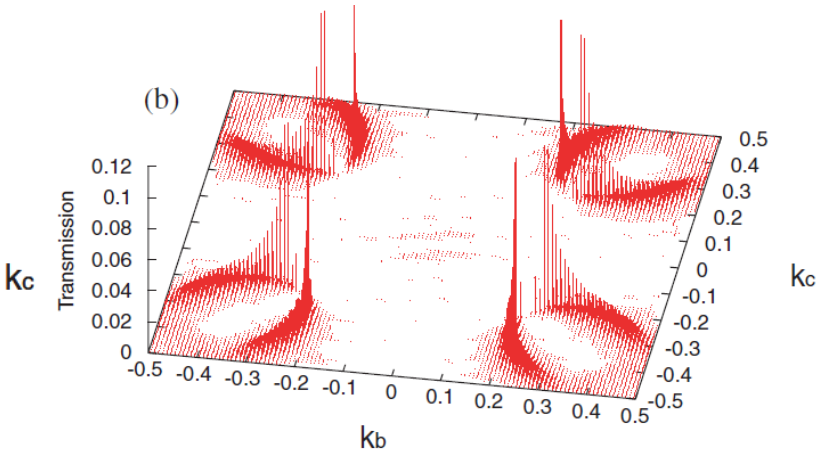
k-dependency of transmission (Fe|MgO|Fe)

up for ↑↑

mainly comes from s-orbital

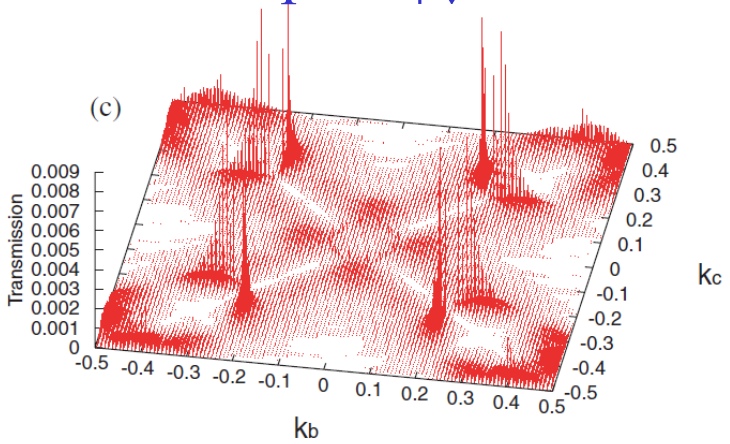


down for ↑↑



mainly comes from d-orbital

up for↑↓



$LaMnO_3/SrMnO_3$

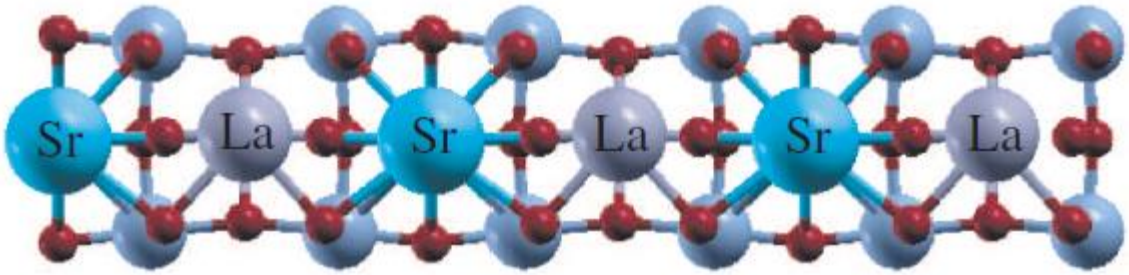
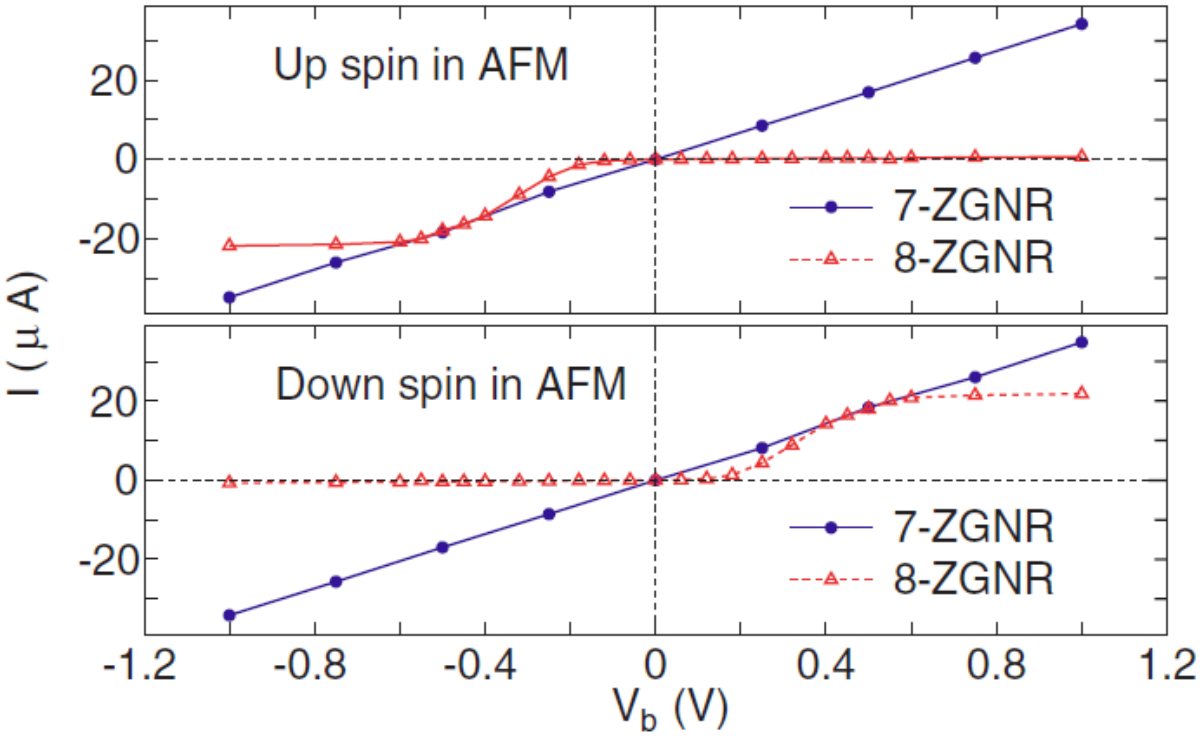


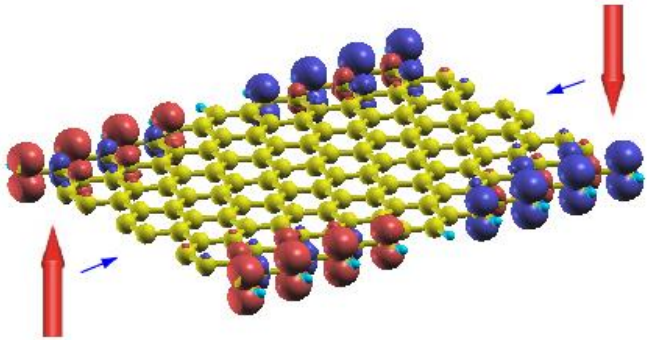
TABLE I: Total energy (meV) per formula unit, $LaMnO_3/SrMnO_3$, and conductance G ($\Omega^{-1}\mu m^{-2}$) of the $(LaMnO_3)/(SrMnO_3)$ supperlattice with four different magnetic configurations, i.e., ferromagnetic (F), A-type (A), G-type (G), and C-type (C) antiferromagnetic configurations of Mn sites. The total energy is measured relative to that of the ferromagnetic configuration. $G_{\uparrow,\mathrm{in}}$ is the in-plane conductance for the up spin state, and the others are construed in the similar way. For the conductance calculations **k**-points of 60×60 were used.

	F	A	C	G
Energy	0	5.0	163.8	248.2
$G_{\uparrow,\mathrm{in}}$	2262	1433	1169	1646
$G_{\downarrow,\mathrm{in}}$	1.82×10^{-2}	1425	1105	1646
$G_{\uparrow,\mathrm{out}}$	1741	664	1127	678
$G_{\downarrow,\mathrm{out}}$	6.43×10^{-3}	655	1128	677

Dual spin filter effect of the magnetic junction

Rectification ratio at 0.4V: 44.3





PRB 81, 075422 (2010).

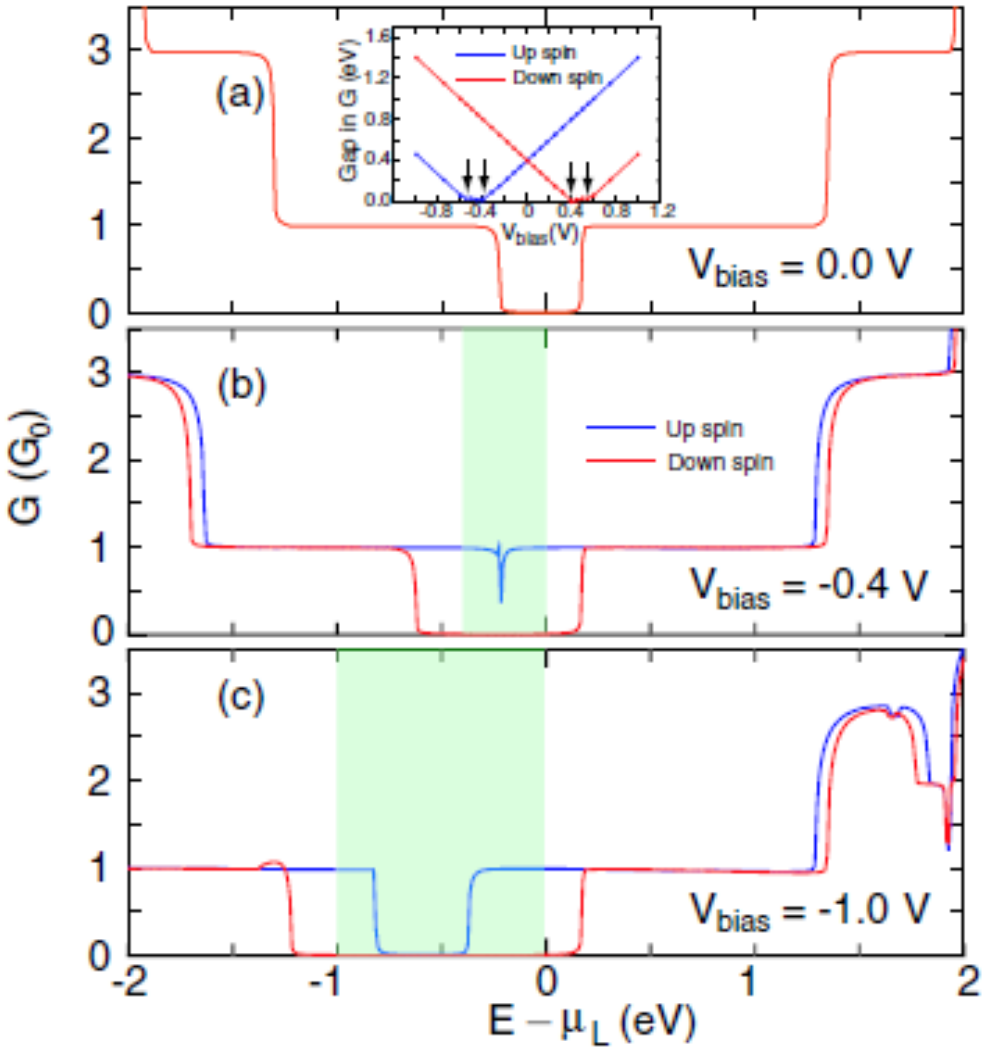
up spin : flowing from right to left

down spin: flowing from left to right

→ Dual spin filter effect

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

Conductance (transmission) of 8-ZGNR



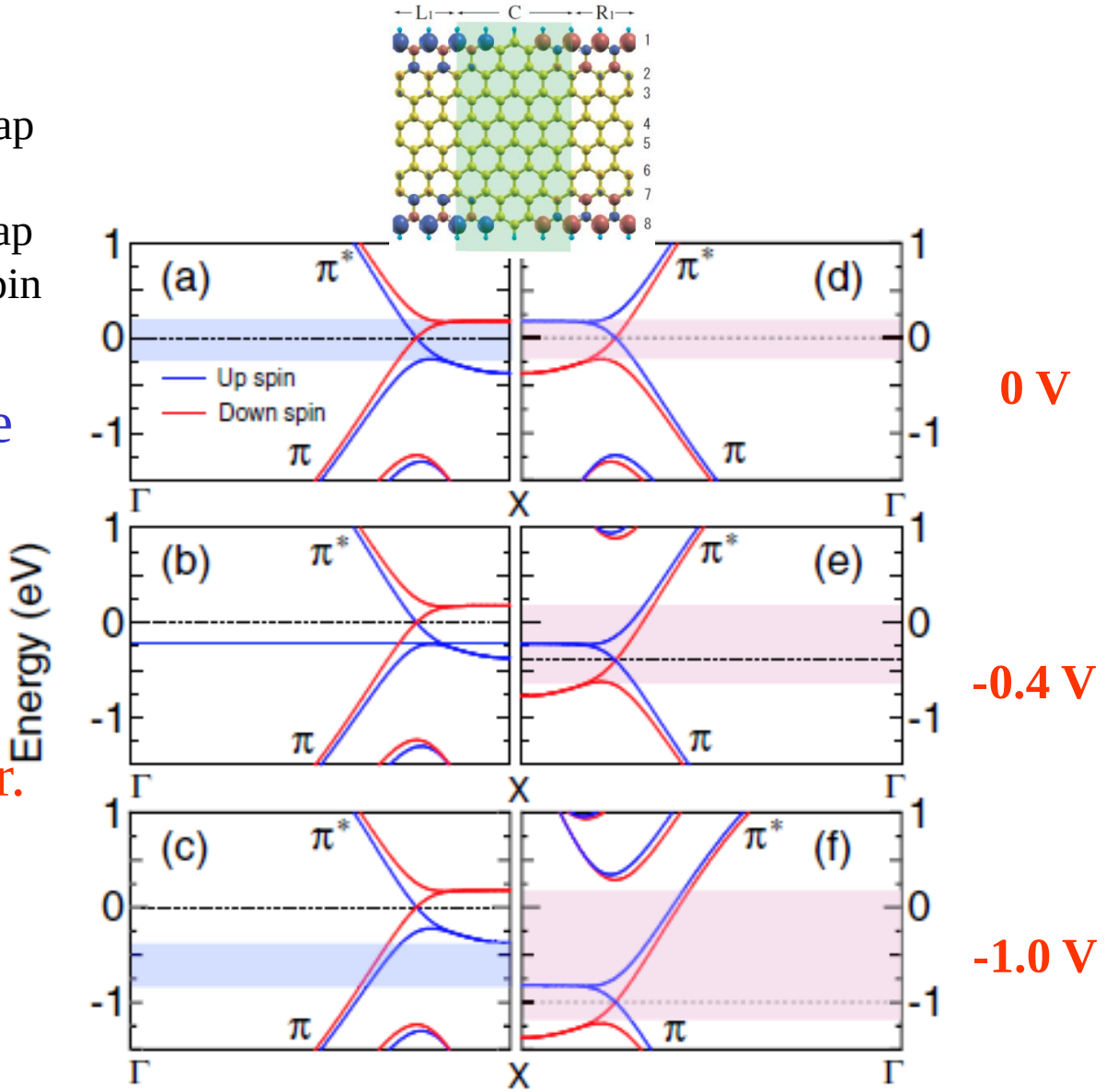
For the up-spin channel, the conduction gap disappears at -0.4 V, while the gap keep increasing for the down spin channel.

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.



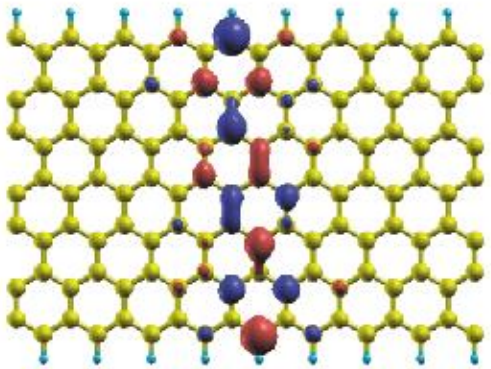
Wannier functions of π and π* states

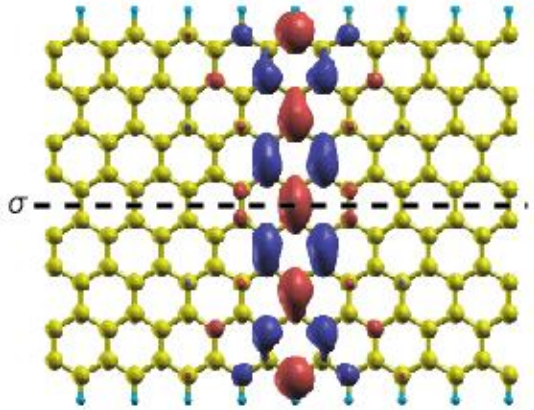
calculated from by Marzari's method

7-ZGNR

8-ZGNR

π^*

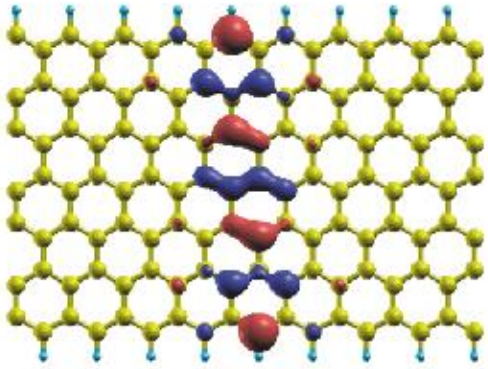


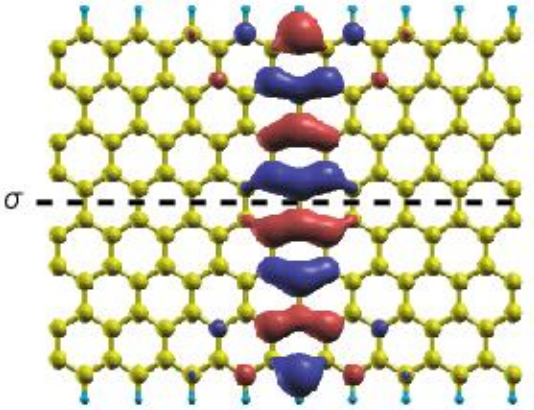


Symmetric

Neither symmetric nor asymmetric

π

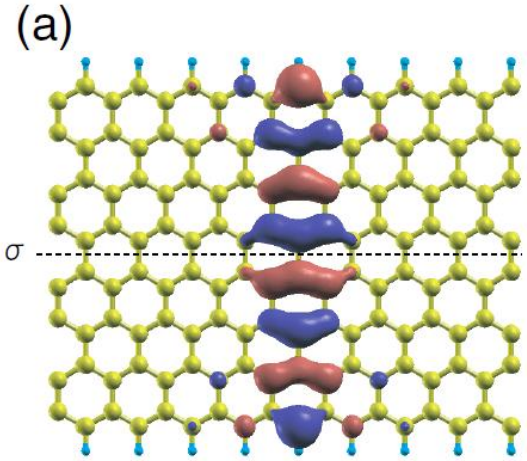




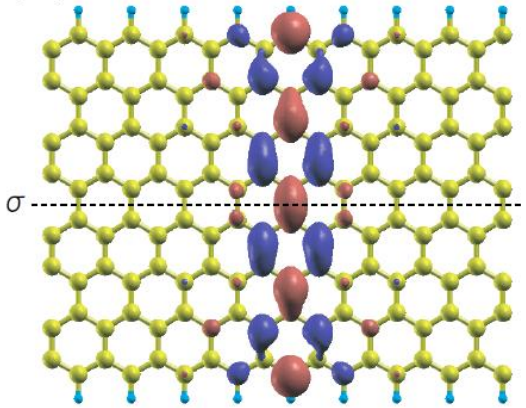
Asymmetric

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

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

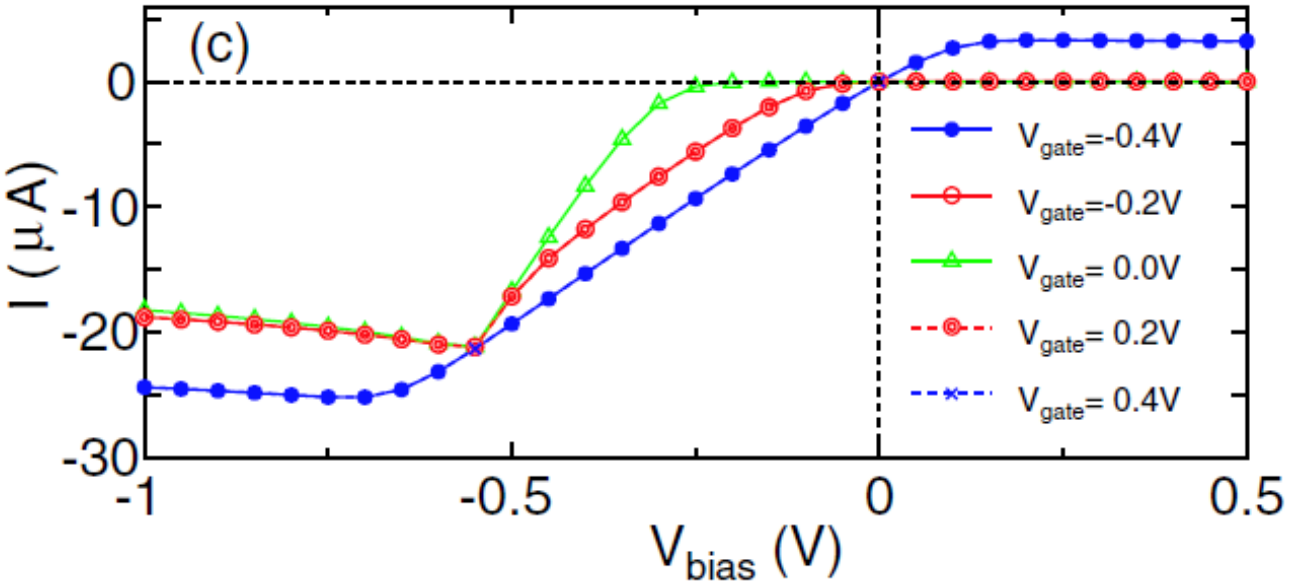
$$T(E) = \frac{4S_L(E)S_R(E)}{[S_L(E) + S_R(E)]^2}$$

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

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

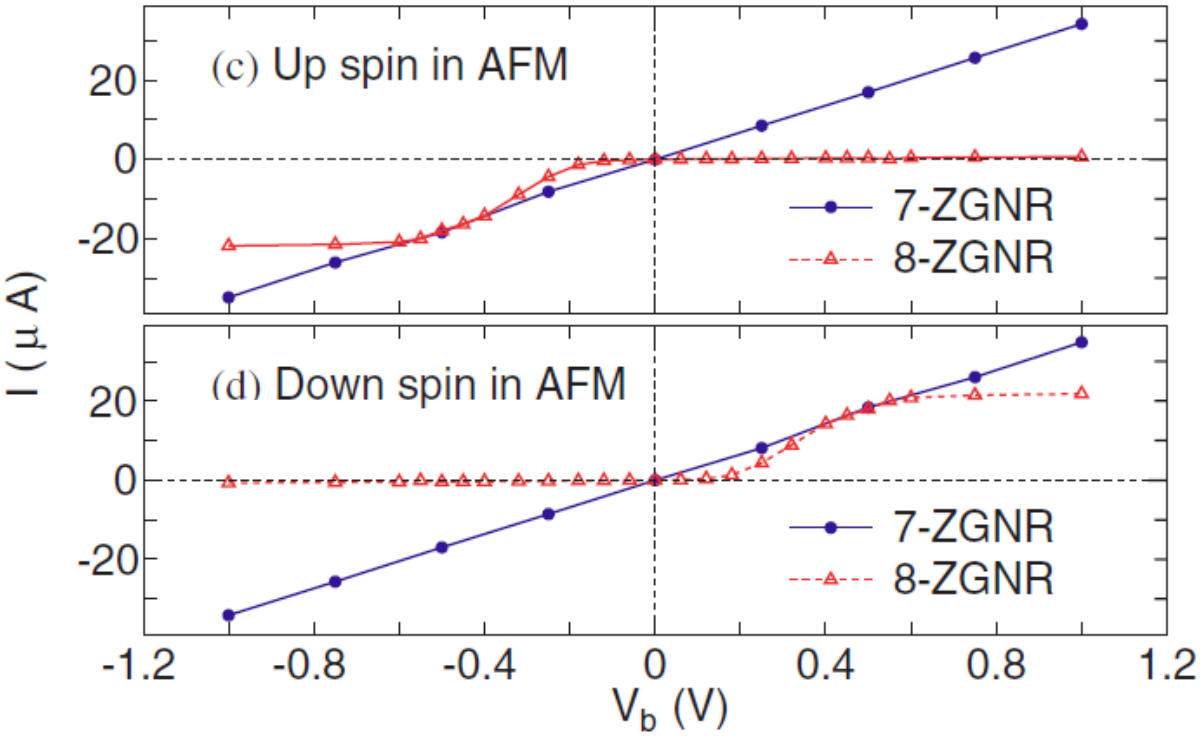
The TB model well reproduces the result of the NEGF calculation.

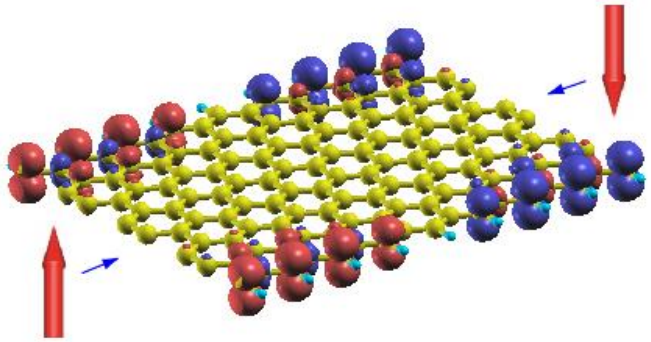
I-V by the simplified TB model



Exercise 4

Reproduce the dual spin filter effect of 8-zigzag graphene nanoribbon discussed in PRB 81, 075422 (2010).





TO et al., PRB 81, 075422 (2010).

Input files are available in work/negf_example for 8-zigzag graphene nanoribbon with an antiferromagnetic junction under a finite bias voltage of 0.3 V.

Step 1: Lead-L-8ZGNR.dat, Lead-R-8ZGNR.dat
Step 2: NEGF-8ZGNR-0.3.dat

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

http://www.openmx-square.org/openmx_man3.8/node113.html

Example 1: carbon chain

Step 1

% ./openmx C1-Lead.dat

Output: C1-CHAIN.hks

Step 2

% ./openmx C18-NEGF.dat

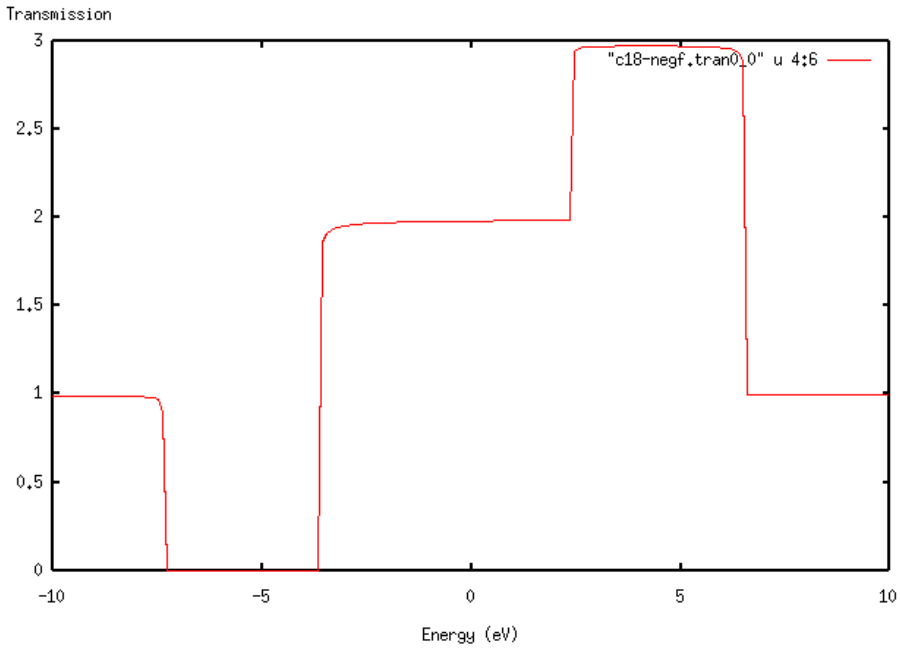
Output: c18-negf.tranb

Step 3

% ./TranMain C18-NEGF.dat

Output: c18-negf.tran0_0, c18-negf.current, c18-negf.conductance

You can get the following transmission by plotting c18-negf.tran0_0.



The input files can be found in work/negf_example

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

Example 2: Graphene

Step 1

% ./openmx Graphene-Lead.dat

Output: Gra-Lead.hks

Step 2

% ./openmx Graphene-NEGF.dat

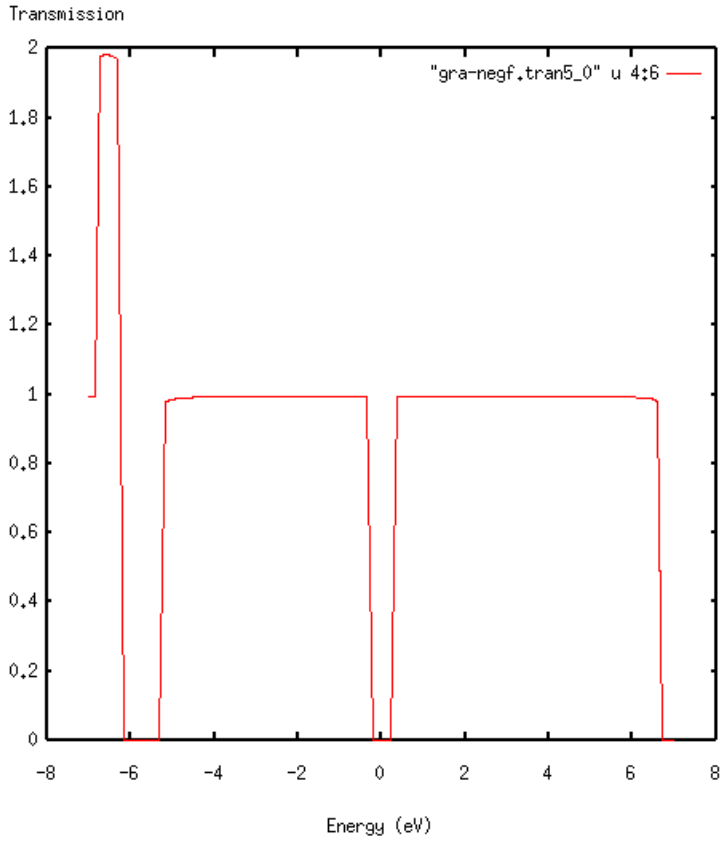
Output: gra-negf.tranb

Step 3

% ./TranMain Graphene-NEGF.dat

Output: gra-negf.tran0_0, gra-negf.tran1_0,…..
gra-negf.current, gra-negf.conductance

You can get the following transmission by plotting gra-negf.tran5_0.



The input files can be found in work/negf_example

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

Summary

The NEGF method combined with DFT provides a general framework for a first-principles treatment of electronic transport problems in a sense that

- Equivalent treatment of lead and scattering region
- Self-consistent treatment under finite bias voltage
- Enabling large-scale calculations
- Inclusion of e-p and e-e interactions via self-energy terms

The method can be applicable to a wide variety of materials including nanowires, superlattices, molecular junctions, and carbon nanotubes.