Current density and eigenchannel: Implementation and application

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STM experiment of eigenchannel on Pb(111) surface

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Eigenchannel analysis on Pb(111) surface

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Current density and eigenchannel

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Outline

• Why eigenchannel and current density?

• Part 1. Eigenchannel on Pb(111) surface
  • Motivation: STM experiment of Pb(111) surface
  • First-principles eigenchannel analysis
  • Result
  • Summary

• Part 2. Implementation of current density in OpenMX
  • Motivation
  • Conventional method for current density
  • Method
    • Current density in NEGF method
    • Difficulty and improvement
  • Result
    • 8-Zigzag Graphene Nanoribbon with domain wall
  • Summary
Motivation

Real-space picture for the conducting phenomena in a nano device

- Eigenchannels
- Real-space current density

OpenMX and Software Advancement project@ISSP
Conductance evolution and tip position


On-top: The first-layer Pb atom lies just under the tip.

hcp: The second-layer Pb atom lies just under the tip.

3 nearest neighbor atoms on the surface.

fcc: The third-layer Pb atom lies just under the tip.

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On-top: The first-layer Pb atom lies just under the tip.

hcp: The second-layer Pb atom lies just under the tip.

3 nearest neighbor atoms on the surface.

fcc: The third-layer Pb atom lies just under the tip.
Eigenchannel in the STM experiment


Superconductor

Cooper pair

ee

e

e

h

h

hh

Superconductor

\[ \frac{2\Delta}{e} \]

\[ \frac{2\Delta}{2e} \]

\[ \frac{2\Delta}{3e} \]
Observed channel and Objective

Fit: Multiple Andreev reflection formula $\rightarrow$ observed $I-V$

Character of each channel (atomic orbital, spatial distribution)

Microscopic picture from a first-principles calculation

fcc vs hcp
Transmission between semi-infinite electrode

\[ \hat{G}_C(E) = \{ E - \hat{H}_C - \hat{\Sigma}_L(E) - \hat{\Sigma}_R(E) \}^{-1} \]

\[ \hat{\Sigma}_L(E) = (E - \hat{H}_{CL})\hat{G}_{LL}(E - \hat{H}_{LC}) \]

\[ \rho(r) = \frac{i}{2\pi} \int_{-\infty}^{\infty} dE \left[ G_C(r, r, E + i0) - G_C(r, r, E - i0) \right] f(\mu - E) \]

\[ \hat{H}_C \]

\[ V_{KS}(r) \]

\[ \rho_{\text{periodic}}(r) \]
Conductance and eigenchannel theory

\[ J = \int \frac{dE}{2\pi} \text{Tr}[\hat{T}(E)]\{f(E - \mu_L) - f(E - \mu_R)\} \]

\[ \hat{T}(E) = \hat{G}_C(E)\hat{\Gamma}_L(E)\hat{G}_C^+(E)\hat{\Gamma}_R(E) \]

Nearly zero bias \( \rightarrow \)

\[ J \propto \text{Tr}[\hat{T}(0)](\mu_L - \mu_R) \]

Eigenchannel

M. Paulsson and M. Brandbyge, PRB 76, 115117 (2007).

\[ \hat{T}(E)|t_i(E)\rangle = t_i(E)|t_i(E)\rangle \]

\[ \text{Tr}[\hat{T}(E)] = \sum_i t_i \]

Visualize transmission path
Numerical procedure and condition

(1) Structure optimization of slab model (periodic)
- Optimize yellow region only
- Super cell of $4 \times 4 \text{Pb}(111)$ unit (48 atoms, Hex)

(2) Electrode (periodic)

(3) Device green’s function

Numerical conditions
- OpenMX (Localized basis set + Pseudo potential) (Project for advancement of software usability@ISSP)
- GGA–PBE functional
- $k$ points: $2 \times 2 \times 1$ (1), $2 \times 2 \times 200$ (2), $2 \times 2$ (3)
- Smearing: 1600 K (0.01 Ry)
- Basis: Pb8.0–s3p3d3f2 (Empty atoms on surface)
- Ignore Spin–Orbit interaction
Conductance

Transmission probability of each channel

on-top | fcc | hcp

Experiment
Eigenchannels (on-top)

on-top

Result

500 nm

$1^{st}$ channel

$p_z$ like

$2^{nd}$ channel

$p_x$ and $p_y$

330 nm

The same as 330 nm
Eigenchannels (hcp)

hcp

1st channel

500 nm

2nd channel

330 nm

Hybridization with the surface orbital

Result
Optimized structure (height of each layer)

About 4 Å: on-top has narrowest tip-surface
4 Å ~ 3 Å: Attraction of tip-surface

hcp/fcc > on-top
We implemented a function for calculating eigenchannels in OpenMX (Project for advancement of software usage@ISSP).

Conductance and eigenchannels in STM experiment of Pb(111)surface–Pb tip are reproduced semi-quantitatively.

We explained the relation between spatial distribution of eigenchannels and tip–surface structure.
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Current density in nanosystem

\[ J(r) = \frac{i}{2} \sum \left[ \psi_i(r) \nabla \psi_i^*(r) - \psi_i^*(r) \nabla \psi_i(r) \right] \]

Left electrode

Right electrode

C. Li, L. Wan, Y. Wei, and J. Wang, Nanotechnology 19, 155401 (2008).

Correction for the Non-local potential

Hybrid functional

Pseudopotentials

\[ \sum B_{ij} |\beta_i\rangle\langle\beta_j| \]
Conventional method

- Source and drain from electrodes
- Identical to the result of the Landauer formula at the center

In practice, it is hard for OpenMX

Objective: Avoiding this difficulty.

Current density with non-local potential

\[ i \frac{\partial \psi(r, t)}{\partial t} = -\frac{\nabla^2}{2} \psi(r, t) + \int d^3 r ' V(r, r ' ) \psi(r ', t) \quad (1) \]

With non-local potential

\[ \psi^*(r, t) \times (1) - \psi(r, t) \times (1)^* \]

Hybrid functional

\[ -\frac{\partial \rho(r, t)}{\partial t} = \nabla \cdot J_{\text{Loc}}(r, t) + \rho_{\text{NLoc}}(r, t) \]

Pseudopotential

[ \sum B_{ij} |\beta_i \rangle \langle \beta_j| ]


\[ J_{\text{Loc}}(r, t) \equiv \frac{i}{2} [\psi(r, t) \nabla \psi^*(r, t) - \psi^*(r, t) \nabla \psi(r, t)] \]

\[ \rho_{\text{NLoc}}(r, t) \equiv i \int d^3 r ' V(r, r ') \psi(r ', t) \psi^*(r, t) - \text{c.c.} \]

\[ J_{\text{NLoc}}(r, t) \equiv \nabla \cdot \varphi_{\text{NLoc}}(r, t) \]

\[ \nabla^2 \varphi_{\text{NLoc}}(r, t) = \rho_{\text{NLoc}}(r, t) \]

Poisson eq.
Current density in NEGF

Left Electrode

\[ \hat{H}_{CL} \]

\[ \hat{G}_{LL} \]

Central(device)

\[ \hat{H}_{CR} \]

\[ \hat{G}_{RR} \]

Right Electrode

\[ \begin{align*}
\hat{G}_C(E) &= \{ E - \hat{H}_C - \hat{\Sigma}_L(E) - \hat{\Sigma}_R(E) \}^{-1} \\
\hat{\Sigma}_L(E) &= (E - \hat{H}_{CL})\hat{G}_{LL}(E - \hat{H}_{LC})^{-1} \\
J &= \int \frac{dE}{2\pi} \text{Tr}[\hat{G}_C(E)\hat{\Gamma}_L(E)\hat{G}_C(E)\hat{\Gamma}_R(E)]\{f(E - \mu_L) - f(E - \mu_R)\} \\
J_{Loc}(r) &= \sum_{ij} [\hat{G}_C\hat{\Gamma}_R\hat{G}_C]_{ij} [\chi_j(r)\nabla\chi_i(r) - \chi_i(r)\nabla\chi_j(r)] [f(E - \mu_L) - f(E - \mu_R)] \\
\rho_{NLoc}(r) &= -2 \sum_{ij} [\hat{\nabla}\hat{G}_C\hat{\Gamma}_R\hat{G}_C]_{ij} \chi_i(r)\chi_j(r) [f(E - \mu_L) - f(E - \mu_R)]
\end{align*} \]

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

\[ \hat{\Gamma}_L \equiv \text{Im}[\Sigma_L] \]

Total current:

Current density:
Result of the conventional method

Inconsistent with the Landauer formula

Source and drain by the coupling to electrodes
\[ \nabla \cdot J \text{ is given} \]

\[ J(x) = J(0) + \int_0^x dx' \frac{dJ(x')}{dx'} \]

Contribution from this region is ignored
Obtain $\nabla \cdot \mathbf{J}$ through a different route

the continuity equation

$$\frac{\partial \rho(r, t)}{\partial t} = \nabla \cdot \mathbf{J}_{\text{Loc}}(r, t) + \rho_{\text{NLoc}}(r, t)$$

In the steady state

$$\rho_{\text{NLoc}}(r) = -\nabla \cdot \mathbf{J}_{\text{Loc}}(r)$$

Boundary condition for the Poisson eq.

$$J = \int \frac{dE}{2\pi} \{f(E - \mu_L) - f(E - \mu_R)\} \sum_{ij} \left[ \hat{G}_C(E) \hat{f}_L(E) \hat{G}_C(E) \hat{f}_R(E) \right] \int d^2 x_{\perp} \chi_i(r) \chi_j(r)$$


Force identical to the Landauer formula at boundaries

Identical in whole region
8-Zigzag graphene nanoribbon

Numerical conditions
- OpenMX (Software Advancement Project@ISSP)
- LDA-PZ functional
- Norm-conserving PP
- Basis: C5.0-s2p1, H5.0-s2
- PW cutoff (Poisson eq.): 120 Ry
- Smearing: 300 K

Magnetization: $0.24 \mu_B$/edge/cell

- Magnetic moment at edges
- Spin filter effect (Domain wall)

Current density

Localized at edge

Delocalized
Conservation of current density

Local: Effect of non-local potential in the vicinity of C atoms.
Our method: Identical to the Landauer formula at each slice.

Conserved current density
Summary

◆ When we implement the conventional method for the current density into OpenMX, there is a difficulty in the Poisson equation for computing non-local current.

◆ We developed a new method for computing non-local term with the aid of the continuity equation. And we implement this method into OpenMX (Software advancement project).

◆ We applied this method to 8–Zigzag graphene nanoribbon.

◆ Targets
  ◆ (Anisotropic) tunnel magneto-resistance device.
  ◆ Graphene (nanoribbon)
  ◆ SiC
  ◆ Etc…

◆ We can also compute the non-collinear spin current density

\[ J_{\sigma\sigma'}(r) \] 3 × 3 matrix at each spatial point (spin × velocity)
Transmission between semi-infinite electrode

\[
\begin{pmatrix}
\hat{H}_L & \hat{H}_{LC} & 0 \\
\hat{H}_{CL} & \hat{H}_C & \hat{H}_{CR} \\
0 & \hat{H}_{RC} & \hat{H}_R
\end{pmatrix}
\begin{pmatrix}
|\psi_L\rangle \\
|\psi_C\rangle \\
|\psi_R\rangle
\end{pmatrix} = E
\begin{pmatrix}
|\psi_L\rangle \\
|\psi_C\rangle \\
|\psi_R\rangle
\end{pmatrix}
\]

\(\hat{H}_L|\varphi_n\rangle = E|\varphi_n\rangle\)

\[
\begin{pmatrix}
|\psi_L\rangle \\
|\psi_C\rangle \\
|\psi_R\rangle
\end{pmatrix} = \begin{pmatrix}
|\varphi_n\rangle + \hat{G}_{LC}\hat{H}_{CL}|\varphi_n\rangle \\
\hat{G}_C\hat{H}_{CL}|\varphi_n\rangle \\
\hat{G}_{RC}\hat{H}_{CL}|\varphi_n\rangle
\end{pmatrix}
\]

\[
\begin{pmatrix}
\hat{G}_L & \hat{G}_{LC} & \hat{G}_{LR} \\
\hat{G}_{CL} & \hat{G}_C & \hat{G}_{CR} \\
\hat{G}_{RL} & \hat{G}_{RC} & \hat{G}_R
\end{pmatrix} = \left[E - \begin{pmatrix}
\hat{H}_L & \hat{H}_{LC} & 0 \\
\hat{H}_{CL} & \hat{H}_C & \hat{H}_{CR} \\
0 & \hat{H}_{RC} & \hat{H}_R
\end{pmatrix}\right]^{-1}
\]
Detail for calsurating eigenchannel

\[ |t_i(E)\rangle: \text{Special superposition of} \]

\[ \hat{A}_L \hat{G}_C \hat{A}_L^\dagger |t_i\rangle = t_i |t_i\rangle \]

Spectral function

Hermite

\[ \hat{A}_L |a_i\rangle = a_i |a_i\rangle \]

\[ \hat{A}_L^{1/2} \equiv (\sqrt{a_1} |a_1\rangle, \ldots, \sqrt{a_N} |a_N\rangle) \]

\[ \hat{A}_L^{1/2} \hat{A}_L^{-1/2} |t_i\rangle = t_i \hat{A}_L^{1/2} \hat{A}_L^{-1/2} |t_i\rangle \]

In the real space

\[ t_i(r) = [\chi_1(r), \ldots, \chi_N(r)] |t_i\rangle \]

In OpenMX

\[ \int d^3 r \chi_i(r) \chi_j(r) \neq \delta_{ij} \]
The Kohn-Shame eqn. in the non-orthogonal basis space

\[ \hat{H} |\varphi_i\rangle = \varepsilon_i \hat{S} |\varphi_i\rangle \]

Solve directly Generalized Eigenvalue Problem

Löwdin ort.

\[ \hat{H} \hat{S}^{-1/2\dagger} \hat{S}^{1/2\dagger} |\varphi_i\rangle = \varepsilon_i \hat{S}^{1/2} \hat{S}^{1/2\dagger} |\varphi_i\rangle \]

\[ \hat{S} |s_i\rangle = s_i |s_i\rangle \]

\[ \hat{S}^{1/2} = (\sqrt{s_1} |s_1\rangle, \cdots, \sqrt{s_N} |s_N\rangle) \]

\[ \hat{S}^{-1/2\dagger} = (s_1^{-1/2} |s_1\rangle, \cdots, s_N^{-1/2} |s_N\rangle) \]

\[ |\varphi_i\rangle = \hat{S}^{-1/2\dagger} |\tilde{\varphi}_i\rangle \]

Löwdin orthogonalizations
Löwdin ort. for $\hat{G}_C$, $\hat{\Gamma}$, $\hat{T}$, eigenchannels

Hamiltonian
$$\hat{H} = \hat{S}^{-1/2} \hat{H} \hat{S}^{-1/2}$$

Green’s function
$$\hat{G} = \hat{S}^{1/2} \hat{G} \hat{S}^{1/2}$$

Self energy
$$\hat{\Gamma} = \hat{S}^{-1/2} \hat{\Gamma} \hat{S}^{-1/2}$$

Line width
$$\hat{T} = \hat{G}_C \hat{\Gamma}_L \hat{G}_C \hat{\Gamma}_R = \hat{S}^{1/2} \hat{G}_C \hat{\Gamma}_L \hat{G}_C \hat{\Gamma}_R \hat{S}^{-1/2}$$

Any vectors
$$|\varphi_i\rangle = \hat{S}^{-1/2} |\tilde{\varphi}_i\rangle$$

Basis set
$$\tilde{\chi}_n(r) = \sum_n \chi_n(r) \left[ \hat{S}^{-1/2} \right]_{n'n}$$

Obtain it in the orthogonal basis space

$$\hat{T}(E)|\tilde{\epsilon}_i(E)\rangle = t_i(E)|\tilde{\epsilon}_i(E)\rangle$$

Diagonalize in the orthogonal basis space

$$|t_i\rangle = \hat{S}^{-1/2}|\tilde{\epsilon}_i\rangle$$

Transform to the non-orthogonal basis space

Any vectors
$$|\varphi_i\rangle = \hat{S}^{-1/2} |\tilde{\varphi}_i\rangle$$

Basis set
$$\tilde{\chi}_n(r) = \sum_n \chi_n(r) \left[ \hat{S}^{-1/2} \right]_{n'n}$$

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