Boundary-Element Methods For Nanoscale Device Modeling

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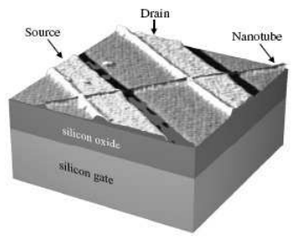
Objective

To predict IV curves from *fully quantum-mechanical* models of actual fabricated nanoscopic electronic devices, such as carbon nanotube FETS.



Methods

1. *Electrostatics:* Given σ on device, and electrode voltages, find electrostatic potential Φ on the device.
2. *Statistical Mechanics:* Given Φ on device, and given electronic density of states in device, find σ on device.
3. *Self-Consistency:* Iterate steps 1 and 2 until Φ and σ have converged.
4. *Landauer/NEGF Transmission Theory:* Given Φ and σ, compute transmission coefficient $T(E)$ & current I.

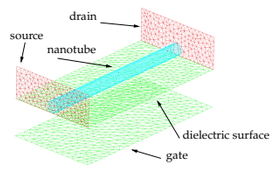
Electrostatics: Φ from σ

Problem: Solve $\nabla^2\Phi = -\frac{\sigma}{\epsilon_0}$ with B.C.s $\Phi(\mathbf{x}) = \begin{cases} V_S, & \mathbf{x} \in \text{ source} \\ V_D, & \mathbf{x} \in \text{ drain} \\ V_G, & \mathbf{x} \in \text{ gate} \end{cases}$

Solution: $\Phi(\mathbf{x}) = \underbrace{\int_{\text{nanotube}} \frac{\sigma(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} dA'}_{\text{known}} + \underbrace{\int_{\text{electrodes}} \frac{\sigma(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} dA'}_{\text{unknown!}}$

Boundary-element method

Introduce panel discretization of electrode and nanotube surfaces; let σ_i and Φ_i be (constant) charge density and potential on ith panel.



Note easy handling of open boundary conditions!

$$\Longrightarrow \Phi_i = \overbrace{\sum_{\text{nanotube panels}} \mathbb{V}_{ij}\sigma_j}^{\text{known}} + \overbrace{\sum_{\text{electrode panels}} \mathbb{V}_{ik}\sigma_k}^{\text{still unknown!}} \qquad \mathbb{V}_{ij} = \text{contribution of charge on panel } j \text{ to potential at centroid of panel } i$$

Find unknown electrode panel charges σ_i by demanding that this equation yield the correct (known) potentials at the panel centroids $\rightarrow$ N_{panels} equations in N_{panels} variables:

$$\vec{\mathbb{V}}_1 \cdot \vec{\boldsymbol{\sigma}}_{\text{EL}} = \vec{\boldsymbol{\Phi}}_{\text{EL}} - \vec{\mathbb{V}}_2 \cdot \vec{\boldsymbol{\sigma}}_{\text{NT}} \Longrightarrow \text{linear system for } \boldsymbol{\sigma}_{\text{EL}} \text{ in terms of } \boldsymbol{\Phi}_{\text{EL}} \text{ and } \boldsymbol{\sigma}_{\text{NT}}!$$

Now use $\boldsymbol{\sigma}_{\text{EL}}, \boldsymbol{\sigma}_{\text{NT}}$ to compute $\Phi(\mathbf{x})$ anywhere in space, *including on the nanotube surface:*

$$\Phi(\mathbf{x}) = \overbrace{\sum_{\text{nanotube panels}} \mathbb{V}_{\mathbf{x}j}\sigma_j}^{\text{known}} + \overbrace{\sum_{\text{electrode panels}} \mathbb{V}_{\mathbf{x}k}\sigma_k}^{\text{now known!}}$$

Statistical Mechanics: σ from Φ

Problem: Find number of electrons per area in a region of potential Φ.

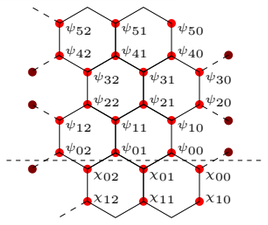
Solution: $\sigma = e\int_{-\infty}^{\mu+e\Phi} \mathcal{D}(E)dE$, $\quad \mathcal{D}(E)$ = nanotube density of states, μ = Fermi level in electrodes

Tight-binding DOS in zigzag carbon nanotubes

Schrödinger:
$[\epsilon_i - e\Phi_i]\Psi_i + t\sum_{\text{neighbors}} \Psi_{i'} = E\Psi_i$

Solution *ansatz:*

$$\psi_{nm} = \begin{cases} e^{ik_m m}e^{ik_n n}, & n = 4q \\ e^{i\frac{k_n}{4}}e^{ik_m m}e^{ik_n n}, & n = 4q+1 \\ e^{i\frac{k_n}{2}}e^{ik_m m}e^{ik_n n}, & n = 4q+2 \\ e^{i\left[\frac{k_n}{2}+\frac{k_n}{4}\right]}e^{ik_m m}e^{ik_n n}, & n = 4q+3 \end{cases}$$

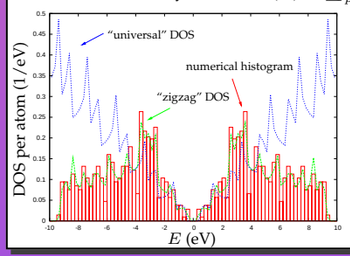


$\Longrightarrow$ Dispersion for pth transverse mode: $E_p(k) = \pm t\sqrt{1+\beta_p^2+2\beta_p\cos 2k}$ $\quad \left(\beta_p = 2\cos\frac{\pi p}{N_1}\right)$

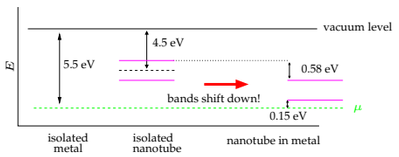
$\Longrightarrow$ Density of states for mode p:

$$\mathcal{D}_p(E) \propto \left|\frac{\partial E}{\partial k}\right|^{-1} = \begin{cases} \frac{|\epsilon|}{\left[4\beta_p^2-(\epsilon^2-1-\beta_p^2)^2\right]^{1/2}}, & |1-|\beta_p|| \le |\epsilon| \le 1+|\beta_p| \\ 0, & \text{otherwise} \end{cases} \qquad (\epsilon = E/t)$$

$\Longrightarrow$ Overall density of states: $\mathcal{D}(E) = \sum_p \mathcal{D}_p(E)$



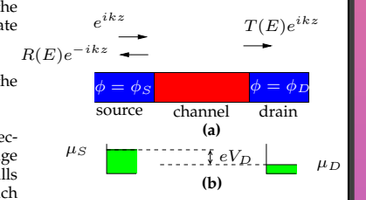
NT inside metal: band shifts



Charge Transport: $T(E)$ from Φ

Landauer Picture of Current Flow

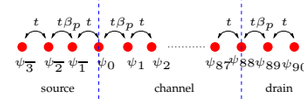
- Electrons of energy E in transverse channel p within the source impinge on the nanotube channel and propagate through to the drain with amplitude $T_p(E)$.
- Similarly, electrons from the drain propagate to the source, also with amplitude $T_p(E)$.
- If both drain and source are equally populated with electrons at all energies, no net current flows. But if a voltage V_D is applied to the drain, then the drain Fermi level falls and an energy window of width eV_D opens in which current flow is uncompensated:



$$I_p = \frac{2e}{\hbar}\int_0^{eV_D} |T_p(E)|^2 \left\{f_{\text{FD}}(E) - f_{\text{FD}}(E+eV_D)\right\} dE.$$

Computing The Transmission Coefficient

- Basic idea: In the source and drain, ϕ is constant, so we may immediately write down the eigenstate of energy E and transverse wavevector p: $\psi \sim e^{ip\varphi}e^{ikz}$, where $k = k_{S,D}(E)$.
- In the channel, ϕ is variable, so we can't write down an analytical solution of Schrödinger's equation, but we can write down an equation relating the amplitudes at adjacent cross-sectional slices in the tube: $[E+e\Phi_i]\psi_i + t\beta_p\psi_{i-1} + t\psi_{i+1} = 0$.
- We take a incoming state $\psi_0 \sim e^{ikz}$ incident from the source, solve numerically for the amplitudes $\psi_1, \psi_2, \cdots, \psi_N$ obtained by propagating this state through the nanotube, and read off the transmission coefficient from the amplitude ψ_N.

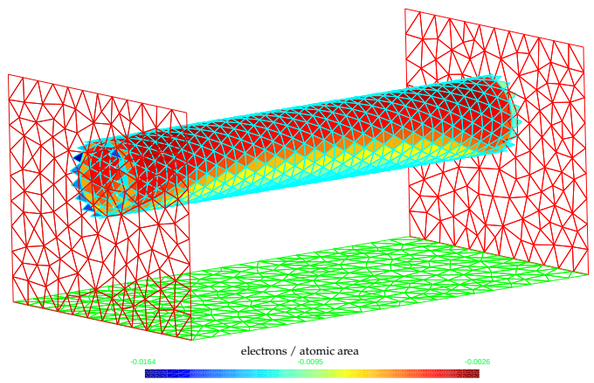


$$\left[E - \overbrace{\mathbf{H}}^{\text{contains } \phi} - \overbrace{\boldsymbol{\Sigma}_S - \boldsymbol{\Sigma}_D}^{\text{"self-energies"}}\right] \cdot \boldsymbol{\Psi} = \overbrace{\boldsymbol{\Gamma}}^{\text{"broadening"}}$$

$\Longrightarrow$ solve linear system for $\boldsymbol{\Psi}$, then set $T_p(E) = \Psi_N$

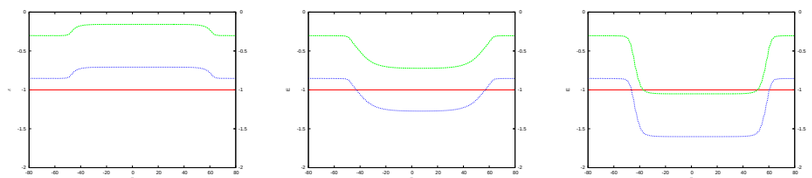
- "Self-energies" and "broadening" are really just fancy names for boundary conditions.

Charge density in a (17,0) zigzag CNTFET, $V_G = -10$ V



Results

Band bending in a (17,0) zigzag CNTFET



$V_G = -4$ V
μ in valence band
current can flow

$V_G = +1$ V
μ in bandgap
current is blocked!

$V_G = +2$ V
μ in conduction band
current can flow

Zero-bias Conductance of a (17,0) zigzag CNTFET