Overview

- Develop theory, approximations and computer code to model quasi 1D structures such as nanotubes, DNA & MOSFETs

- Nanotubes: Influence of defects on ballistic transport, electronic-thermal properties, Metal-nanotube coupling

- DNA: Model electron transfer, spectroscopy and transport experiments, Sequence dependence of conductivity

- MOSFET: Analyze under a variety of conditions

Outline

- What effects are modeled?
- Equations & computational requirements
- Specific Structures considered
- Drain current vs. Gate voltage of a well-tolerated MOSFET

- Evolution of device scale
- Scaling Design and measured energy
- Model validation: experimental data
Model

Neglected:
- Discrete nature of dopant distribution
- Electron-impurity and electron-electronphonon scattering
- Hopping (Kondo)
- Band structure

What do we model

- Anisotropic effective mass equation for electrons
- Carrier injection at source, drain and gate open boundaries
- Ballistic transport
- Source to Drain tunneling
- Gate Tunneling
- Non-Equilibrium Green's function equations (Schrödinger-Poisson solver at both (kT)

Equations

- Equations for retarded (Gr) and advanced (Gk) Green's functions:
  \[ (E-H-T) \Delta G_{\alpha \beta}(r,r';E) = \delta_{\alpha \beta} (\delta(E-E'-E_{\alpha}) ) \]
- \[ \left( \begin{array}{cc}
E - H - T & G_{\alpha \beta}(r,r';E) \\
G_{\alpha \beta}(r,r';E) & (E-H-T) \Delta G_{\alpha \beta}(r,r';E)
\end{array} \right) \Delta = \left( \begin{array}{c}
z_{\alpha} \\
z_{\beta}
\end{array} \right) \]
- \( \Sigma \) represents self-energy due to band-bounded and other scattering mechanisms

Computational requirements

- \[ (E-H-T) \Delta G_{\alpha \beta}(r,r';E) = \delta_{\alpha \beta} (\delta(E-E'-E_{\alpha}) ) \]
- Electron density at \( r \) = \( G(r,r';E) \) - Required receptivity in Poisson's equation
- LxH is Block tridiagonal matrix
- Block size = N
- We require only the diagonal elements of \( G \)
- Developed an algorithm to solve for the diagonal blocks of \( G \)
- Number of operations \( N \times (N+1) \)
- \( N \times N \) of mesh and points \( (N \times N) = N \times a \times b = N \times n \times m \) of mesh and points
- Full block version
- Full block algorithm
- Exact self-energy for the entire scatterng region
- Diagonalization of the entire system
- Realistic model of the entire system

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Future Challenges:

• Increased role of tunneling and quantized levels in the channel of nanoscale MOSFET requires a better treatment of bandstructure
  • project underway: applying the 2D code to study transport in CNT with 4-orbital tight-binding Hamiltonian, which looks structurally the same
• Quantitative models for scattering are required
  • scattering time comparable to flight time
  • discretization of kz-space
• Hole band is required for pMOS
• Better algorithms are needed to solve NEGF equations
  • Need diagonal elements of Gr and G< rather than blocks