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-structural properties: Metal-semiconductor coupling, diffusion.
- DNA: Model electron transfer, biochemistry, and transport experiments. Sequence dependence of conductance.
- MOSFETs: Charge transport and current-voltage behavior.
- Source codes available in FORTRAN and C.

Outline

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

- Evolution of transport under different conditions
- Drain current vs. Gate voltage at various energies
- Model transport measurements
Model

Neglected:
- Discrete nature of dopant distribution
- Electron-impurity and electron-electron/phonon scattering
- HAMPTON
- 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 biases)

Equations

- Equations for retarded (Gr) and lesser (G<) Green\'s functions:
  - (E-H-E) \( G^{\text{r}}(x,r,E) = \Sigma \) (\( G^{\text{r}}(x,r,E) \)
  - (E-H-E) \( G^{\text{l}}(x,r,E) = \Sigma \) (\( G^{\text{l}}(x,r,E) \)
  - \( \Sigma \) represents self-energy, due to band boundaries and other scattering mechanisms

Computational requirements

- (E-H-E) \( \Sigma^{\text{r}}(x,r,E) \)
- Electron density at \( r = \Sigma^{\text{r}}(x,r,E) \) - Required frequency in Poisson\'s equation
- LHB is Block tri-diagonal matrix
- Block size = \( N_x \)

We require only the diagonal elements of \( \Sigma^{\text{r}} \).

Developed an algorithm to solve for the diagonal blocks of \( \Sigma^{\text{r}} \):
- Number of equations \( N_x \cdot N_y \cdot N_z \)
- \( N_x \cdot N_y \cdot N_z \): no. of vectors and points
- \( N_x \cdot N_y \cdot N_z \): no. of spatial and points

For each \( \Sigma^{\text{r}} \) block:
- Communication between processors
- Synchronization of individual processors
- Overlap of communication and computation
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