Green’s Function Approach
For MOSFETs

Ramesh Venugopal

School of Electrical and Computer Engineering
Purdue University

J. Rhew
S. Goasguen
Prof. S. Datta
Prof. M. Lundstrom
CE Group
• Introduction
• Ballistic Electron Transport: *Real vs. Mode Space*
• Boundary Conditions
• Scattering in n-channel MOSFETs
• Summary
Introduction

- **Charge Centroid Shift**
  - Decreases the effective gate capacitance
  - Decreases the on-current

- **Thin Body Effects**
  - Increases the threshold voltage (and fluctuations)
  - Decreases the off-current
  - Decreases the on-current

- **Oxide Tunneling**
  - Increases the off-current

- **Source Barrier Tunneling**
  - Increases the off-current (imposes a scaling limit)

- **Quantum Mechanical Treatment of Scattering**

- **Bandstructure(Strain)/ Heterostructures**
Outline

• Introduction

• Ballistic Electron Transport: Real vs. Mode Space

• Boundary Conditions

• Scattering in n-channel MOSFETs

• Summary
Real vs. Mode Space

- $\Sigma$: Self Energy (Describes Coupling)
- $G^n, G^p$: Correlation Functions (Local Charge Density)
- $\Sigma^{in}, \Sigma^{out}$: The in and out scattering functions (can be related to the state lifetime of electrons and holes)
Real vs. Mode Space

- Basis is \( \delta(x - x') \delta(z - z') e^{ik_y Y / \sqrt{W}} \)
- Single band, multi valley effective mass eqn.
- Bandstructure is linked to grid morphology
  \[ E(k_x) = \frac{\hbar^2}{2m_x} (1 - \cos(k_x \Delta_x)) \]
- Quantum Mechanics (Dyson’s eqn.)
  \[ (E[k_x, k_z]I - H - \Sigma^R)G^R = I \]
- Non-local Carrier Dynamics
  \[ G^n = G^R \Sigma^{in} G^A \quad G^P = G^R \Sigma^{out} G^A \]
- Physical observables along the diagonals
- Block tridiagonal nature of \( H \), permits a recursive calculation of diagonal blocks of \( G \)
- Self energy matrices are perturbative elements
Real vs. Mode Space

\[ G = \left[ EI - H_{Device+Lead} \right]^{-1} = \begin{bmatrix} EI - H_{Device} & \tau \\ \tau^+ & EI - H_{Lead} \end{bmatrix}^{-1} \]

\[ G_{Device} = \left[ EI - H_{Device} - \Sigma_{Lead} (E) \right]^{-1} \]

\[ \Sigma_{Lead} (E) = \tau G_{Lead} \tau = \tau G_{Lead}^{11} \tau^+ \]

\[ I = G_{Lead}^{11} \left[ EI - H_{Lead}^{11} - \tau G_{Lead}^{11} \tau^+ \right]^{-1} \]

- Potential is invariant looking into the lead
- The size of the self-energy matrix is the same as that of the Hamiltonian
- The only non-zero block of the self-energy corresponds to the column of nodes that constitute the boundary between the active device and the lead
• Mode self-energy is $\tau e^{ika}$
• Mode occupancy is limited by the Fermi Function
• Thin body and confinement effects are correctly captured
• Modes can be treated classically or quantum mechanically
Real vs. Mode Space

- Single band, multi valley, effective mass equation.
- Basis is $\delta(x - x')\Psi(x, z)e^{ikY/\sqrt{W}}$
- The overall wavefunction in the $(X, Z)$ plane is $\Phi(x, z) = \sum_i C_i(x)\Psi_i(x, z)$
- The 1D equation that is discretized, is an equation for $C_i(X)$
- Individual modes are treated independently in the Ballistic limit
- Each mode couples to a contact with its unique self-energy
- Treatment of few, decoupled subbands (occupancy limited) greatly reduces computational cost as compared to real space solution
- The problem size is $\sim Nx^2$ as opposed to $\sim (NxNy)^2$
**Real vs. Mode Space**

**Single Subband**

- $T_{Si} = 1.5 \text{ nm}$
- $T_{OX} = 1.5 \text{ nm}$
- $L_G = 10 \text{ nm}$
- $V_{DD} = 0.6 \text{ V}$
- $V_t = 0.15 \text{ V}$
- $S/D = \text{Abrupt}$
- $N(S/D) = 10^{20}/\text{cm}^3$
Real vs. Mode Space

- Mode-Space solutions capture vertical quantum effects
- Quantum effects along the channel are accounted for by coupling modes to contacts
- The 2D spectral function from Real Space simulations includes the mode/subband picture

$V_{GS} = V_{DS} = 0.6V$
Real vs. Mode Space

- Coupling to contacts broadens the 2D DOS and shifts the subband energies
- Local oscillations in charge density/DOS are due to quantum interference
- Local oscillations in charge density are washed out when solving Poisson’s eqn.

$V_{GS} = V_{DS} = 0.6V$
• Mode space solutions are computationally efficient and offer an attractive simulation scheme for modeling SOI devices

• Tunneling affects both the on and the off currents

• ~25% of the on-current is due to tunneling carriers
Real vs. Mode Space

- Self-Consistent Boltzmann solutions in Mode space overpredict the on-current as thermionic carriers have a higher velocity than tunneling carriers.

- When comparing transport models, Selfconsistency solutions must be considered.

- The Mode Space, Boltzmann solution cannot capture source barrier tunneling.
Real vs. Mode Space

Mode space expansion and approximation

• Basis is $\delta(x - x')\Psi_i(x, z)e^{ik_y \sqrt{W}}$ and the wavefunction is $\Phi(x, z) = \sum_i C_i(x)\Psi_i(x, z)$

• Expand the 2D Hamiltonian to evaluate $\langle i \mid H \mid \Phi \rangle$

\[
\begin{bmatrix}
-\frac{\hbar^2}{2m_x} \frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_z} \frac{\partial^2}{\partial z^2} + U(x, z)
\end{bmatrix} \Phi(x, z) = E_L \Phi(x, z)
\]

\[
-\frac{\hbar^2}{2m_x} \frac{\partial^2}{\partial x^2} C_i(x)
\]

\[
\frac{\partial \psi_i(x, z)}{\partial x} = 0
\]

\[
\langle i \mid j \rangle = \delta_{ij}
\]

\[
\frac{\partial}{\partial x} \psi_i(x, z) = 0
\]

• Final 1D equation for mode “i” is

\[
\begin{bmatrix}
-\frac{\hbar^2}{2m_x} \frac{\partial^2}{\partial x^2} - E_i(x)
\end{bmatrix} C_i(x) = E_L C_i(x)
\]
• When modes abruptly change shape the Real and decoupled Mode Space solutions no longer match

• The reduced current from the Real Space solution is due to a quantum mechanical spreading resistance

• Treating the flared out portions of the Source/Drain is challenging
Real vs. Mode Space

The key approximation in the Mode Space Solution:
• The shape of the mode does not vary along the channel, $\frac{\partial \Psi_i(x, z)}{\partial x} = 0$

Implications:
• Different modes are decoupled in the Ballistic Limit
• This solution is justified in case of thin body, fully depleted DG MOSFETs

Computational Complexity: $N_X \times N_Z = 122 \times 10$, $E_{steps} = 1500$
Real Space: $1500*122*10^{2.7}$ flops * 10 (Poisson iterations) ~ 0.9 Gflops
Mode Space (2 modes) = $1500*2*122*\log(122)$ flops* 10 ~ 0.02 Gflops
• Mode space solutions treat few confined modes as higher modes are empty
• Real space solutions implicitly include coupling and all confined modes
• Introduction

• Ballistic Electron Transport: *Real vs. Mode Space*

• Boundary Conditions

• Scattering in n-channel MOSFETs

• Summary
Boundary Conditions

Suppression of the drain injected carriers with increasing drain voltage prevents the source end from attaining charge neutrality in the ballistic limit.

- The artificial n++ region is used to simulate a large scattering contact.
Boundary Conditions

- Floating BC, captures the effect of coupling to a scattering contact
- Floating BC means, $\hat{X} \cdot \nabla V = 0$
- Charge neutrality (Integrated doping equals the integrated charge density) is always realized
Outline

• Introduction
• Ballistic Electron Transport: *Real vs. Mode Space*
• Boundary Conditions
• Scattering in n-channel MOSFETs
• Summary
Scattering

- Electrons are scattered, thermalized, and re-injected.
- Current is conserved through the entire channel.
- The interaction energy between the probe and the device can be related to a mobility

**Energy Relaxation**: Electron energies are fully randomized at each probe (energy relaxation)

\[ \int I(E_L) \, dE_L = 0 \]

**Phase Breaking**: Complete loss of coherence \( I(E_L) = 0 \)
\[ \Sigma(E_L), \] describes the coupling between the probe and the device and can be related to a low field mobility

\[ \Sigma^{\text{in}}(E_L), \text{ and } \Sigma^{\text{out}}(E_L), \text{ are the in and out scattering strengths. They are expressed in terms of } \Sigma(E_L) \text{ and the Fermi-level, } \mu, \text{ of each probe (includes degeneracy)} \]

Current at each probe is constrained to be zero by adjusting Fermi energies of all probes

\[ H = -\frac{\hbar^2}{2m^*} \nabla^2 + U \]

\[ G(E_L) = [E_L I - H - \Sigma(E_L)]^{-1} \]

\[ G^n(E_L) = G(E_L) \Sigma^{\text{in}}(E_L) G^+(E_L) \]

\[ G^p(E_L) = G(E_L) \Sigma^{\text{out}}(E_L) G^+(E_L) \]

\[ I_m(E_L) = \frac{q}{h} \text{Trace} [\Sigma^{\text{in}} G^p - \Sigma^{\text{out}} G^n] \]
Scattering

How does the voltage drop?

- Uniformly doped ($1 \times 10^{20}\text{cm}^{-3}$), semiconductor, 10 mV bias
- The scattering model smoothly scales to the Ballistic Limit
**Scattering**

---

**Ideal absorbing contact to flared out S/D**

**Single Subband**

\[
\begin{align*}
T_{Si} &= 1.5 \text{ nm} \\
T_{OX} &= 1.5 \text{ nm} \\
L_G &= 10 \text{ nm} \\
V_{DD} &= 0.4 \text{ V} \\
S/D &= \text{ Abrupt} \\
N(S/D) &= 10^{20}/\text{cm}^3
\end{align*}
\]

**Multiple Subband**

\[
\begin{align*}
T_{Si} &= 3 \text{ nm} \\
T_{OX} &= 1.5 \text{ nm} \\
L_G &= 10 \text{ nm} \\
V_{DD} &= 0.4 \text{ V} \\
S/D &= \text{ Abrupt} \\
N(S/D) &= 10^{20}/\text{cm}^3
\end{align*}
\]
Scattering

Phase Breaking vs. Energy Relaxing

Reduced Current, Momentum Relaxation
(1.5nm transistor, on-state)

Reduced Current, Energy Relaxation
(1.5nm transistor, on-state)

Ballistic Components, Scattering Components

- Phase breaking scattering does not relax the directed longitudinal carrier energy
Only a small cone of carriers with enough longitudinal energy can make it back to the source.

This cone reduces as one progresses towards the drain thus reducing the probability of backscattering into the source.

• The probability of backscattering from the channel into the source reduces towards the drain

• The high 1D density of states below the source barrier aids downscattering as opposed to upscattering in longitudinal energy

• As the number of subbands increases, band to band coupling causes the backscattering probability is reduced even more
Scattering

Phase Breaking (--) vs. Energy Relaxing

- The phase breaking model exhibits no critical scattering region. Scattering occurring in the entire channel equally affects device performance.

- The energy relaxing model exhibits a critical scattering region wherein scattering strongly affects device performance (Captures the Essential Physics).
Scattering

Coherent vs. Incoherent Transport

- Coherent oscillations in the Local Density of States is washed out due to scattering
- The probe self-energy cuts off below the band edge and there is very little increase in tunneling current due to scattering
Scattering

Potential Drop and Resistance

10mV drain bias 1.5 nm body

- The total resistance is the area under the resistance/square curve

- There are five components to the overall intrinsic device resistance: Source, Drain, Tip, Channel and the Quantum Contact resistance

- In short channel MOSFETs, the tip resistance dominates the overall resistance, although the junctions are abrupt

\[ R \left( \Omega / \text{sq} \right) = \frac{1}{I} \frac{\partial F_{\text{Pr abe}}}{\partial x} \]
Summary

• The Mode Space approach is a computationally efficient and accurate method for simulating quantum transport.

• The decoupled Mode Space method is limited to simulating transport in uniform SOI geometries.

• When coupled with a Büttiker probe based scattering model, the Mode Space solution clearly captures the essential physics of scattering including Fermi degeneracy effects.

• This tool can be used to examine design issues which affect the performance of nanoscale transistors operating in the quasi-ballistic limit.