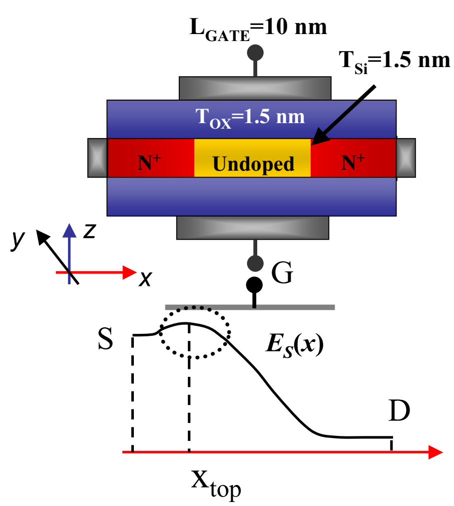
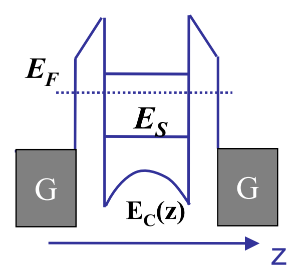
Electron Devices at the Nano/Molecular Scale
Mar. 21-22, 2002
Summer School at UIUC

Semiclassical Transport in nanoMOS

I. Introduction
II. Ballistic BTE
III. Macroscopic Models (DD/ET)
IV. Benchmarking Study
V. Quantum Potential Approaches
VI. Summary

I. Introduction: Physical Picture





- Quasi-2D Approach
  - Quantum in vertical direction
  - Semiclassical along channel
  - Gate charge control

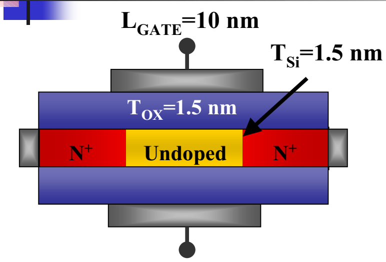
I. Introduction: Motivation/Objectives

- Why Semiclassical in Nanoscale
  - Valid down to L = 10 nm [Ren, Rhew]
  - Continuation of existing approaches (characterization/modeling)
  - Computationally less expensive than quantum
- What to address
  - Essential physics of nanotransistors
  - Validity of conventional macroscopic models (DD/ET/HD)
  - Challenges to new macroscopic models

II. Ballistic BTE: Introduction

- Scaling down $\rightarrow$ Approaching ballistic limit
  - GaAs HEMTs (1980s)
  - Nanoscale MOSFETs (recently)
- To understand
  - Ballistic transport in transistor structures
  - Its implications to nanotransistor modeling
- Key theories
  - State occupancy in the ballistic limit [Datta]
  - Essential physics of nanoscale MOSFETs [Lundstrom]

II. Ballistic BTE: How to Solve

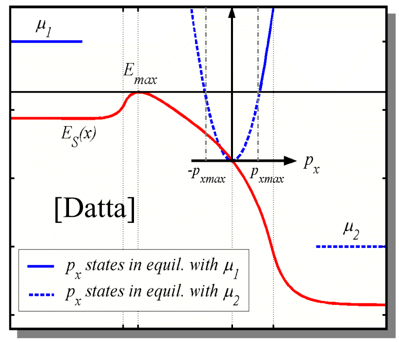


- Equation

$$v_x \frac{\partial f_B(x,\vec{p})}{\partial x} - q\mathcal{E}_x \frac{\partial f_B(x,\vec{p})}{\partial p_x} = 0$$

- Solution

$$f_B(x,\vec{p}) = f_o\left(\frac{p_x^2}{2m^*} + \frac{p_y^2}{2m^*} + E_S(x) - \mu\right)$$

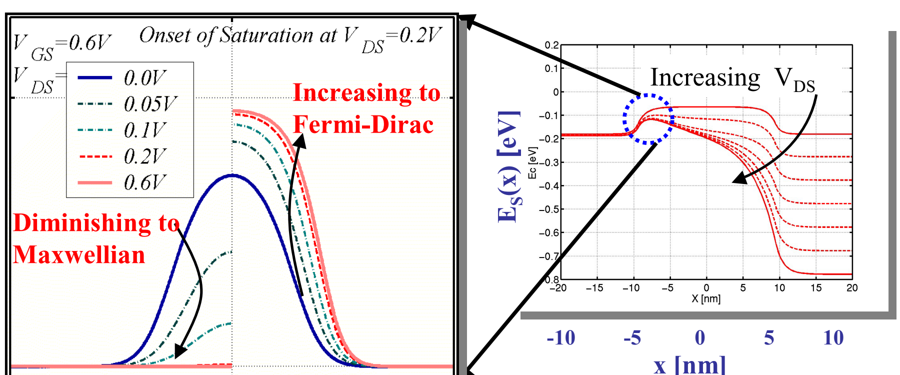


- Boundary Conditions

$$f_B(x=0,\vec{p}) = f_o(E(0,\vec{p});\mu_1),\ p_x > 0$$

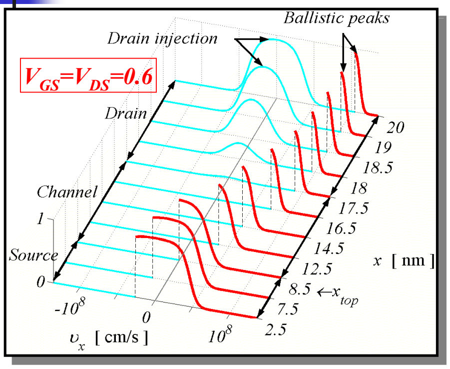
$$f_B(x=L,\vec{p}) = f_o(E(L,\vec{p});\mu_2),\ p_x < 0$$

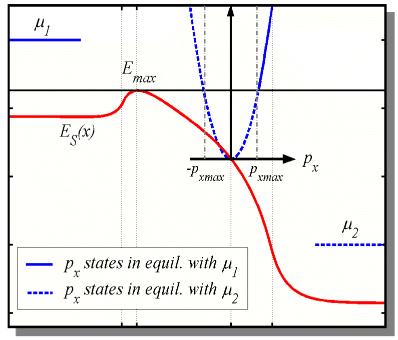
II. Ballistic BTE: At the Source Barrier



Essential Physics (Lundstrom, 1997)
Failure of Macroscopic Models (Nekovee, 1992)

II. Ballistic BTE: Along the Channel





- **Source: Cooling**
- **Top of the barrier: Essential physics**
- **Channel: Ballistic peak**
- **Drain: Heating**

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II. Ballistic BTE: Summary

- Physics of Ballistic Transport
  - Solution of the ballistic BTE
  - Essential physics
  - Ballistic Distribution
    - Equilibrium shape at the barrier
    - Ballistic peaks
- Implications to Nanotransistor Modeling
  - Failure of conventional macroscopic models
  - Challenges to new macroscopic models
    - Impose thermal injection limit
    - Describe ballistic peaks

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III. Macroscopic Models: Drift-Diffusion

- Equations

$$\frac{dJ}{dx} = 0 \qquad J = q\mu_n n\mathcal{E} + qD_n\frac{dn}{dx}$$

- Mobility Model

$$\mu_n = \frac{\mu_0}{\left[1+(\mu_0\mathcal{E}/\upsilon_{sat})^{\beta}\right]^{1/\beta}}$$

- DD vs. Bude's Model

$$DD: \begin{cases} \upsilon_{sat} = 1.0\times10^7\, cm/s \\ \beta = 2 \end{cases}$$

$$Bude: \begin{cases} \upsilon_{sat} = 2.2\times10^7\, cm/s \\ \beta = 1 \end{cases}$$

Discretiztion: Scharfetter-Gummel (SG) scheme

III. Macroscopic Models: Energy Transport

ET models are in Medici flavor

- Current Equations

$$J = q\mu_n(T_n)n\mathcal{E} + q\frac{d}{dx}\left[nD_n(T_n)\right] \qquad D_n(T_n) = \frac{kT_n}{q}\mu_n(T_n)$$

- Energy Equations

$$\frac{dS}{dx} = \frac{1}{q}J\mathcal{E} - n\frac{k}{q}\frac{T_n - T_0}{\tau_E} \qquad S = -\frac{5}{2}\frac{kT_n}{q}\left[\frac{J}{q} + \mu_n n\frac{d}{dx}\left(\frac{kT_n}{q}\right)\right]$$

- Mobility Model

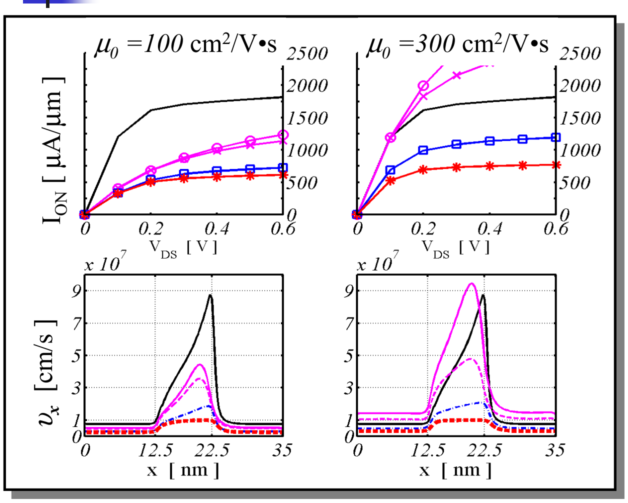
$$\mu_n(T_n) = \frac{\mu_0}{\sqrt{1+\left[\frac{\mu_0}{\upsilon_{sat}^2\tau_E}\frac{k(T_n - T_0)}{q}\right]^2}}$$

Current: SG scheme
Energy: Direct scheme
(Bank & Rose Newton)
Decoupled method

VI. Benchmarking: Introduction

- Reported Problems of Conventional Models
  - DD underestimates I_{ON} [Bude]
  - Advanced models overestimate I_{ON} [Banoo]
- To Identify
  - Limitations of conventional models
  - Challenges to new models
- Benchmarking DD/ET against the Ballistic BTE
  - From diffusive to near-ballistic: μ_0=0 ~ 500 cm^2/Vs
  - Compare I-V and velocity profiles
  - Compare I_{ON} vs. μ_0 and υ_{inj} vs. μ_0

VI. Benchmarking: I-V, Velocity Profiles



ET: τ_E=0.3ps (o)
τ_E=0.1ps (x)

DD (*)

Bude (square)

Ballistic

ET: τ_E=0.3ps (—)
τ_E=0.1ps (---)

DD (---)

Bude (-.-.-)

Ballistic

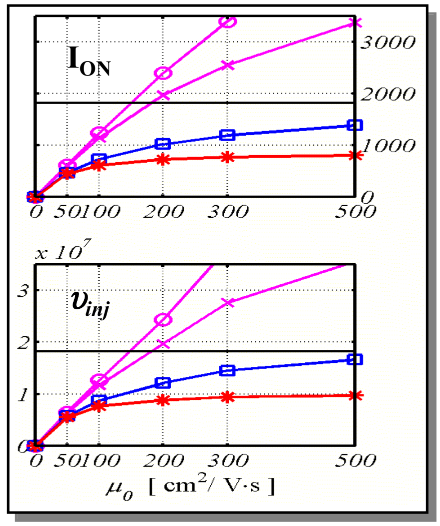
VI. Benchmarking: I_{ON}, υ_{inj} vs. μ_0

ET: τ_E=0.3ps (o)
τ_E=0.1ps (x)

DD (*)

Bude (square)

Ballistic



VI. Benchmarking: Summary

- Limitations
  - DD Model
    - Underestimates near-ballistic I_{ON}
  - Bude's DD Model
    - Reasonable
    - Parameters are not predictive
    - Velocity clamped at υ_{sat}
  - ET Model
    - Exceeds the Ballistic I_{ON} and υ_{inj}.
- Common Reasons for Failure
  - No thermal injection limit is imposed
  - Incorrect description of channel velocity overshoot

V. Quantum Potential: Basic Formulas

- DG formalism: (Wigner's function)

  Using carrier-density-related quantum potential V_{eff} to substitute classical V in conventional Drift-Diffusion equation to capture quantum effects:

$$V_{eff} = V + 2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} \quad \textit{where} \quad b_n = \hbar^2 / \left(4qr_n m_n^*\right)$$

- EP formalism: (Wave Packet Appr.)

  The quantum potential V_{eff} an electron feels is the average value within a wave packet (V_{eff} is not coupled with n directly):

$$V_{eff}(x) = \frac{1}{\sqrt{2\pi a_0}} \int V_{classical}(x+y) \exp\left(-\frac{y^2}{2a_0{}^2}\right) dy$$

  where a_0 is the characteristic size of a wave packet

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V. Quantum Potential: Comparison

Density-Gradient (DG) and Effective-Potential (EP) Models

- S/D tunneling effects for nanoMOS 1D transport models
- EP: all transport models
- DG: conventional macroscopic models only (DD/ET).
- Each model has its own merits/demerits.
- The detailed results and the releasable version of the code will be available soon.

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IV. Summary

- Semiclassical Transport Models in nanoMOS
  - Ballistic BTE
  - DD Models
  - ET Models
- Benchmarking Study
  - Limitations of conventional models
  - Reasons for the failure
- Quantum Potential Approaches
  - Extend the scope of semiclassical models.