Quantum Device Simulation

30A MOS CV Curve – Quantum Currents – and PHEMTs
Introduction

- Why a Quantum Mechanical based simulator is necessary
- Introduction to QM issues and theory
- Implementation and syntax
- Practicalities of use
- Examples (MOS, PHEMT, Diode)
Introduction (con’t)

- Why Use a QM simulator
  - Reduction in device size => coherence length of electrons
  - Thin gate oxides => CV shift
  - Channel sheet carrier shift => MOS/HEMT
  - Heterojunction tunneling
  - Pulse doping ‘smear’
Quantum Issues

- Quantization “carrier confinement”
  - 1D/2D/3D => Quantum Well/Wire/Dot
  - Schrödinger’s Equation
    \[
    -\left(\frac{\hbar^2}{2m^*} \frac{d^2}{dy^2} + V(y)\right) |ψ(y)\rangle = E_i |ψ(y)\rangle
    \]
  - Eigen Value Problem
Quantum Issues (con’t)

- Results appear as a sequence of
  - Eigen energies => Discrete energies where electrons may reside
  - Eigen functions => Probability distribution of electrons along each slice
- Schrodinger -Poisson => Spacial distribution of electrons to replace classical one
Quantum Issues (con’t)

- Transport
  - Transmission, Deflection
  - Concentration
- Quantum corrections to standard transport equations
- Provided by Quantum moments equation
  \[ U_q = -\frac{\hbar^2}{8m}\nabla^2 \ln(n) \]
- Based on second moments of the Wigner distribution function
- Quantum Temperature => Quantum diffusion term
- Bohm Quantum Potential
Implementation and Syntax

- **Schroedinger-Poisson Solver**
  - models Schrodinger Eigens =15

- **Quantum Moments**
  - models quantum
  - solve qx.damp=1.0

- **Bohm Quantum Potential**
  - BQP
Electrostatic Potential, Classical and Quantum Electron Concentrations

Figure 1.
Eigen Wave Functions and Energy Levels

Figure 2.
Figure 3.
Figure 4.
Figure 5.
Figure 6.
Classical and Quantum Electron Concentrations

Figure 7.
Classical and Quantum Currents

Figure 8.
PHEMT – Zero Bias Case

Figure 9.
Figure 10.
Model Comparison

ATLAS
Electron density near GaAs/AlGaAs interface

Electron concentration (log10/cc)

Distance from interface (microns)

AlGaAs
GaAs

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Conclusion

- As a device dimensions shrink, quantum effects become more significant.
- Schrödinger-Poisson solve provides calculations of bound state energies, carrier wave functions and carrier concentrations.
- Quantum effects included in carrier transport by using quantum moments models.