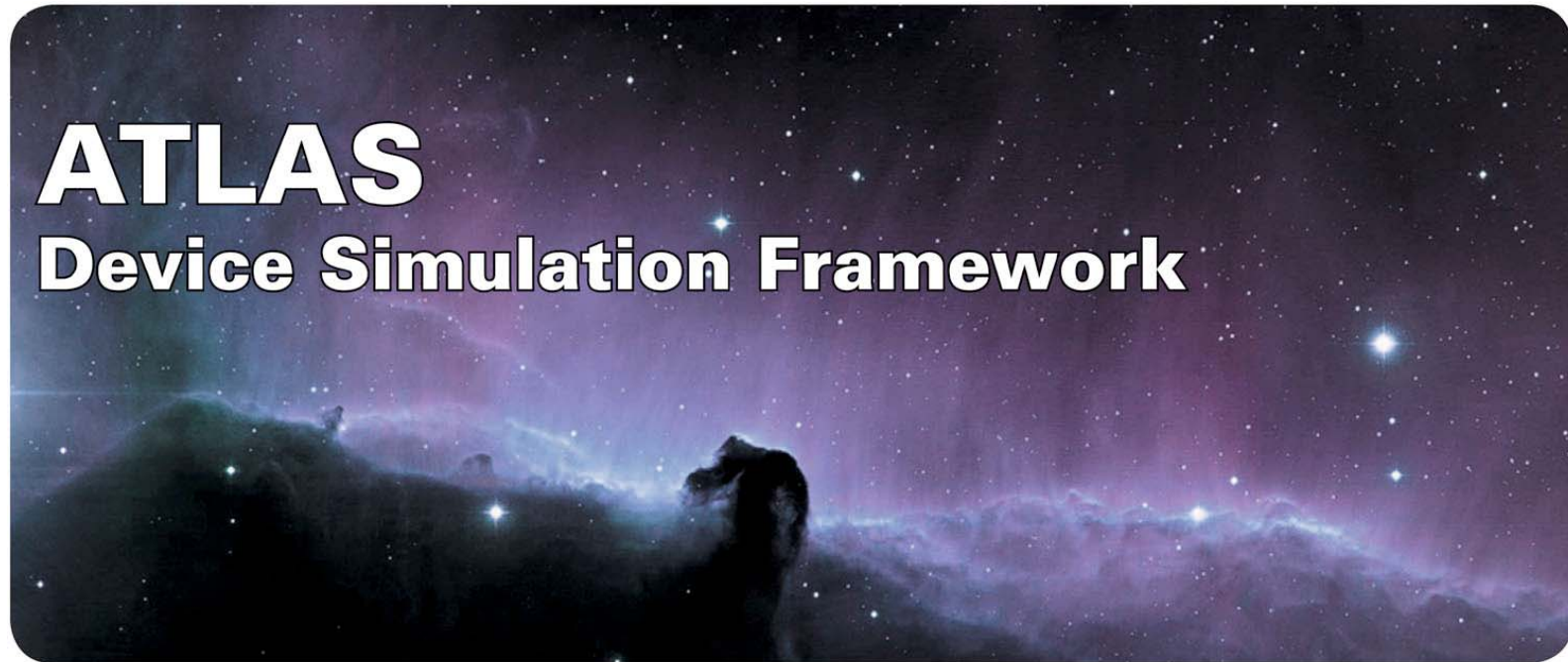


Quantum Device Simulation



Overview Of ATLAS Quantum Features



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Introduction

- Motivation for using Quantum models
- Overview of ATLAS Quantum features
- Discussion of Quantum models



Motivation

- Reduction in device size -> coherence length of electrons
- Thin gate oxides -> Capacitor-Voltage shift, C_{ox} , V_t
- Carrier distribution near interfaces and delta doping not accurately described by classical models
- Tunneling in heterojunctions and Schottky junctions



Device Technologies

- Many technologies have developed with noticeable quantum effects
- MOS - electron distribution near thin gate oxides
- HEMT, HBT, heterojunction barrier diode etc.
- SOI structure with silicon films of few nm
- Quantum Well lasers, VCSELs, LEDs and photodetectors



Overview

- Five separate Quantum Models
 - 1 - Self-Consistent Schrodinger-Poisson Model
 - 2 - Quantum Moments Model
 - 3 - Bohm Quantum Potential
 - 4 - Hansch Quantum Correction Model
 - 5 - Van Dort Quantum Correction Model

- Three Thermionic Emission and Tunneling models
 - 1 - Heterojunction
 - 2 - Schottky contact
 - 3 - Direct gate oxide tunneling

- Quantum Well light emission models



Self-Consistent Schrodinger-Poisson Model

- One dimensional Schrodinger equation solved along y mesh
- Alternating Schrodinger and Poisson equations solved, ie. decoupled but self-consistent
- Eigen-energies and eigenfunctions solved
- Fermi-Dirac statistics used



Self-Consistent Schrodinger-Poisson Model

- syntax:

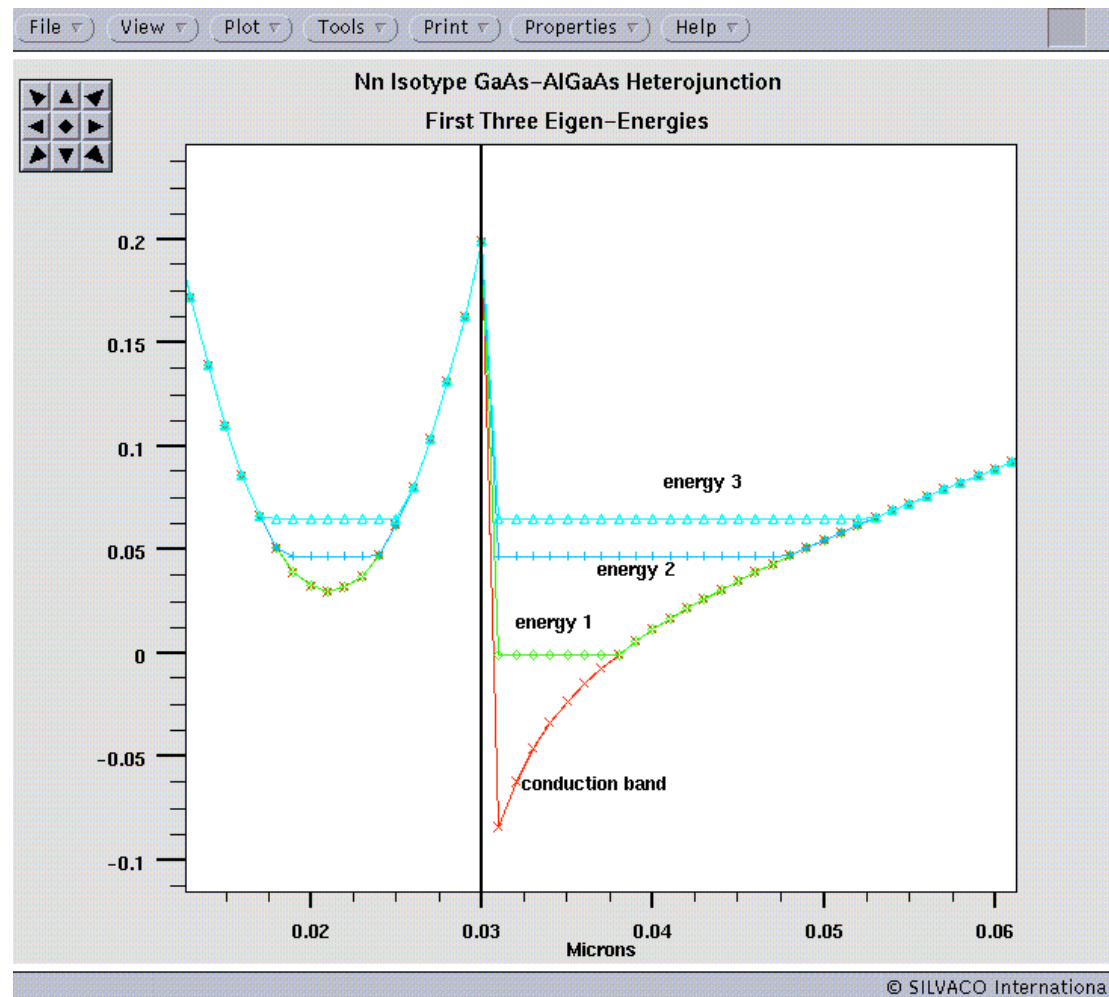
```
MODEL SCHRO
```

```
OUTPUT EIGEN=N // N is an integer
```

```
METHOD CARRIERS=0 // no carrier continuity
```



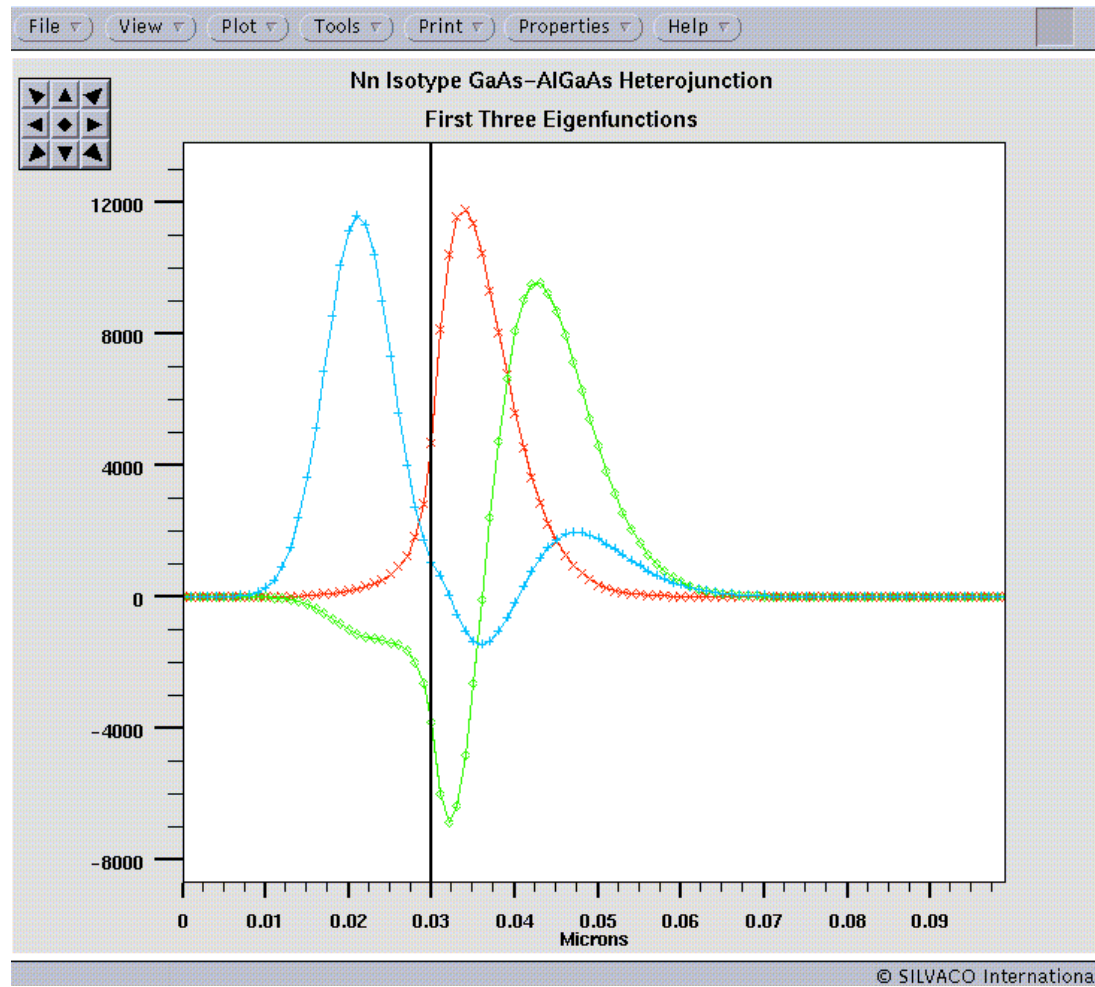
Self-Consistent Schrodinger-Poisson Model



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Self-Consistent Schrodinger-Poisson Model





Non-Self-Consistent Schrodinger Carrier Continuity Model

- Alternately, can solve non-self-consistent solution to include carrier continuity equations
- User control of quasi-Fermi level calculation
- Syntax:

```
MODEL SCHRO POST.SCHRO ^FIXED.FERMI CALC.FERMI //  
Boolean parameters  
METHOD CARRIERS=2 // include carrier continuity
```
- Depending on the application, device and bias range, some combinations of FIXED.FERMI and CALC.FERMI may give unphysical results. Recommendation is to use FIXED.FERMI and CALC.FERMI both TRUE.



Definition of Quasi-Fermi Parameters with Schrodinger /Poisson

FIXED.FERMI	CALC.FERMI	Quasi-Fermi level Calculation method
FALSE	FALSE	Quasi-Fermi level is calculated from the local electron density via drift-diffusion model
FALSE	TRUE	Quasi-Fermi level varies with Y position and is calculated to match the local classical and quantum mechanical charge concentration
TRUE	FALSE	Quasi-Fermi level is uniformly zero
TRUE	TRUE	Quasi-Fermi level is uniform across Y slice and is calculated to match the classical and quantum mechanical sheet charge.

Table 1. Interpretations for post-processed Schrodinger solution.

(Table 3-53 of ATLAS manual - clarification)

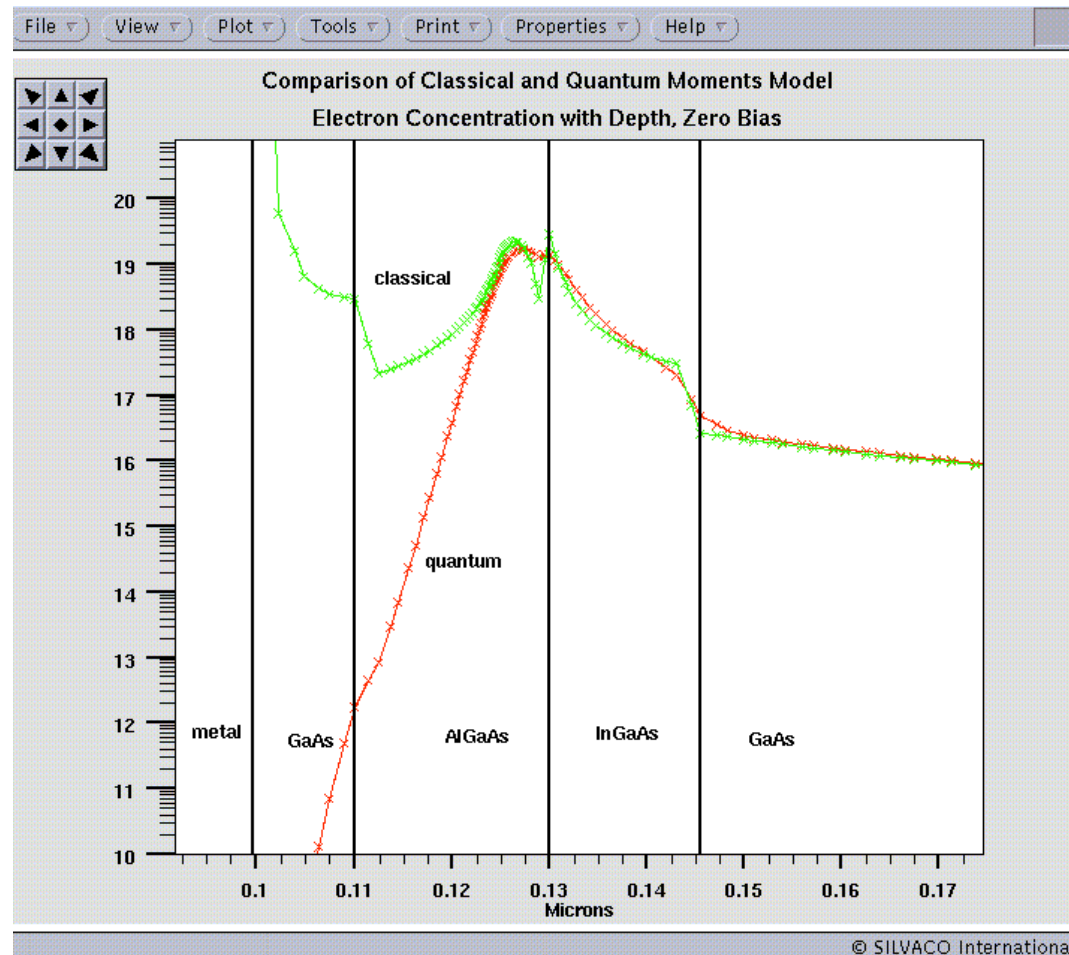


Quantum Moments Model

- Based on Wigner function equations of motion
- Used with 1 or 2 carrier solutions to obtain currents
- Quantum correction to the carrier statistics in current and energy flux equations
- Affects calculated values of carrier concentration near Si/SiO₂ interfaces in MOS and heterointerfaces in HEMTs.
- Syntax:
MODEL QUANTUM H.QUANTUM
//electons and holes, respectively
- Damping factor for convergence and tuning, QFACTOR, ramp to unity
- Quantum moments model also available in 3D

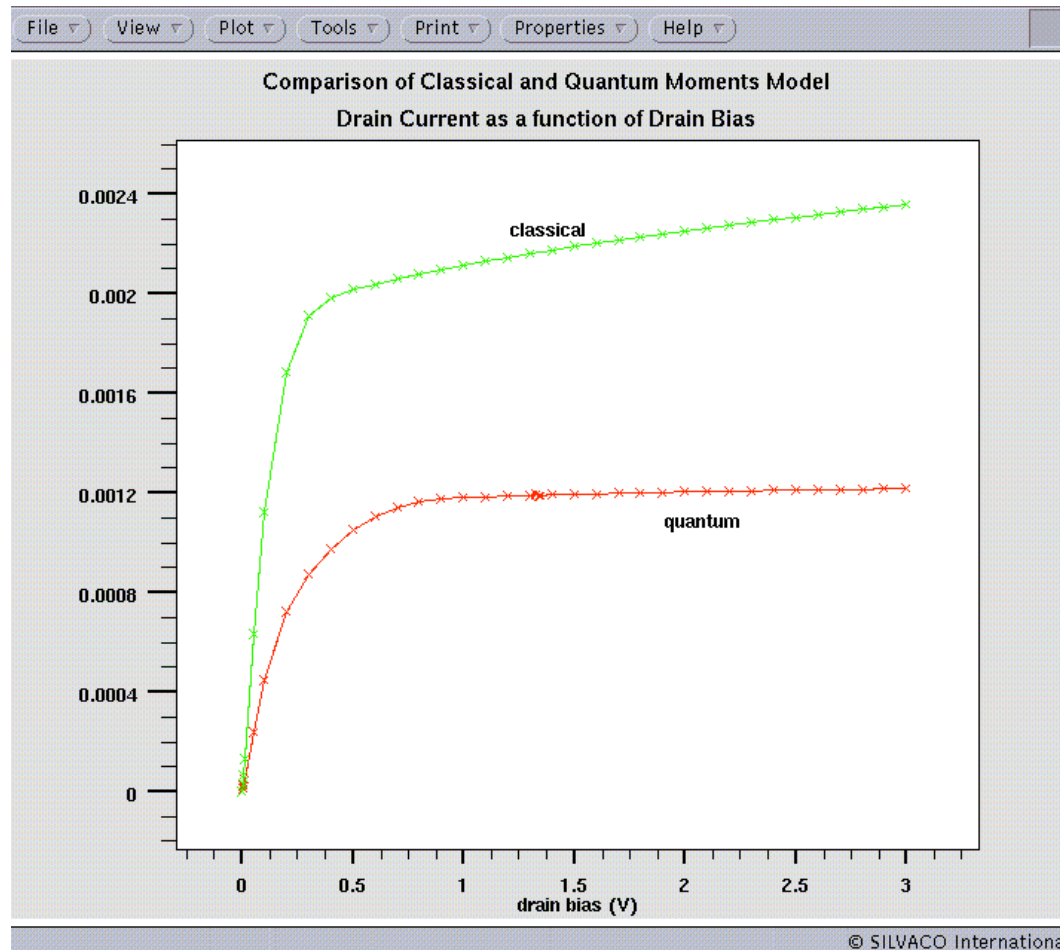


Quantum Moments Model



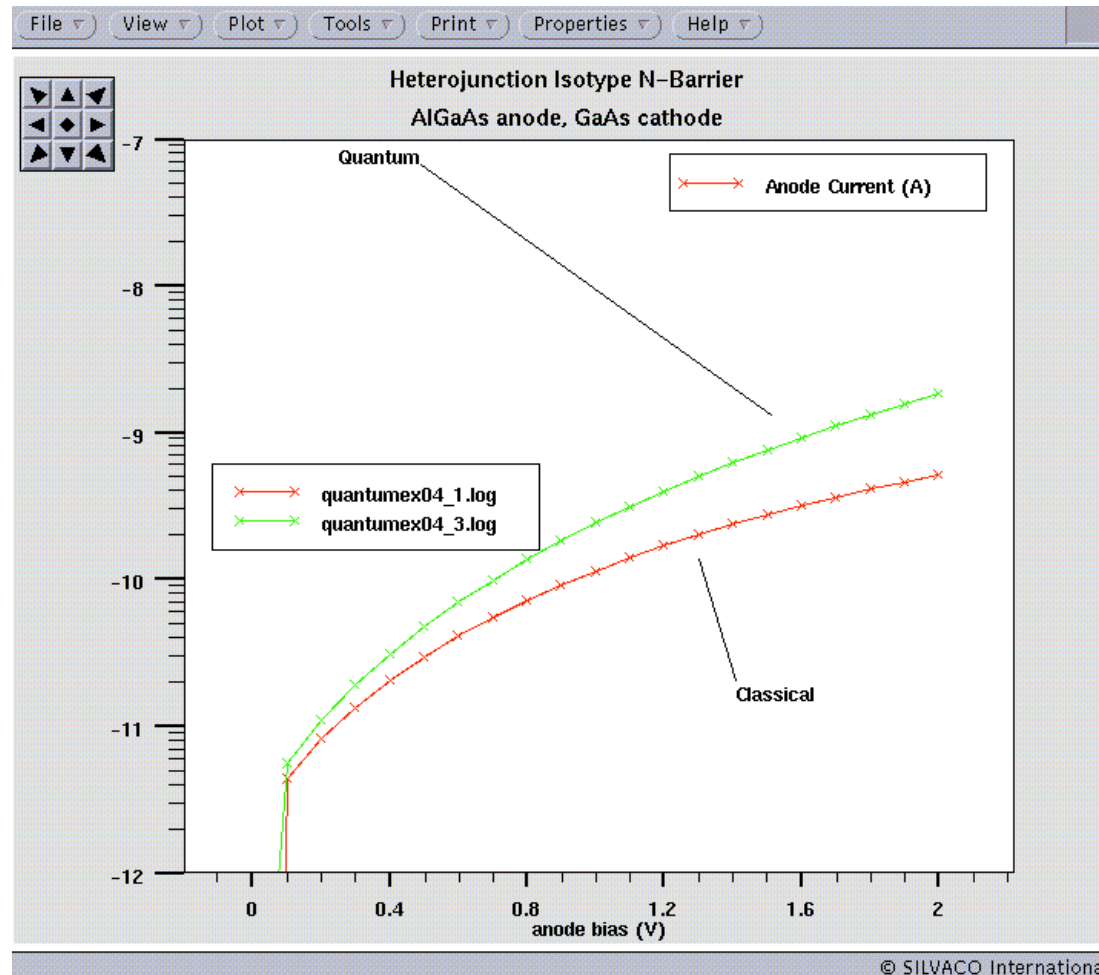


Quantum Moments Model





Quantum Moments Model



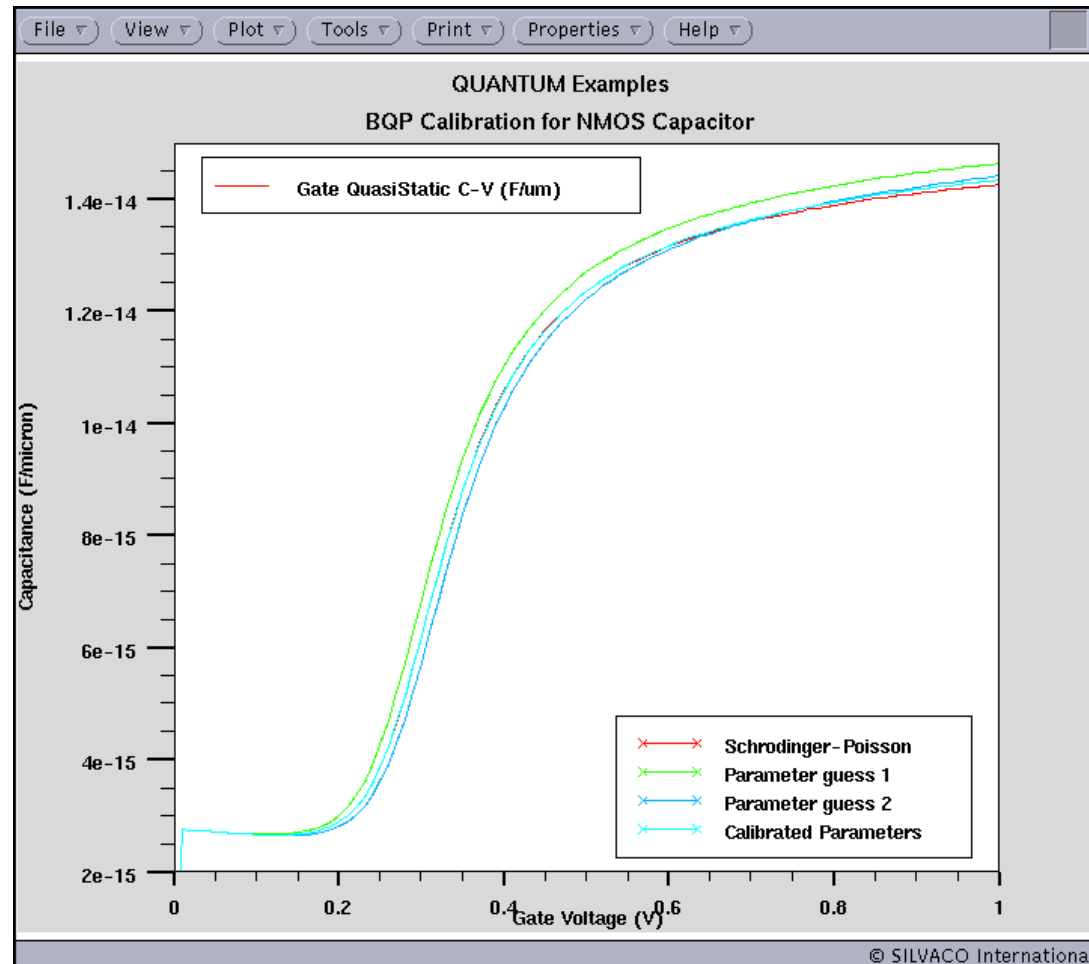


Bohm Quantum Potential (BQP)

- 1 and 2 carrier solutions
- Syntax:
 Model BQP.N BQP.P
- Works with hydrodynamic energy balance models
- 3D
- Better convergence than Quantum Moments Model
- Better calibrated to Schrodinger-Poisson

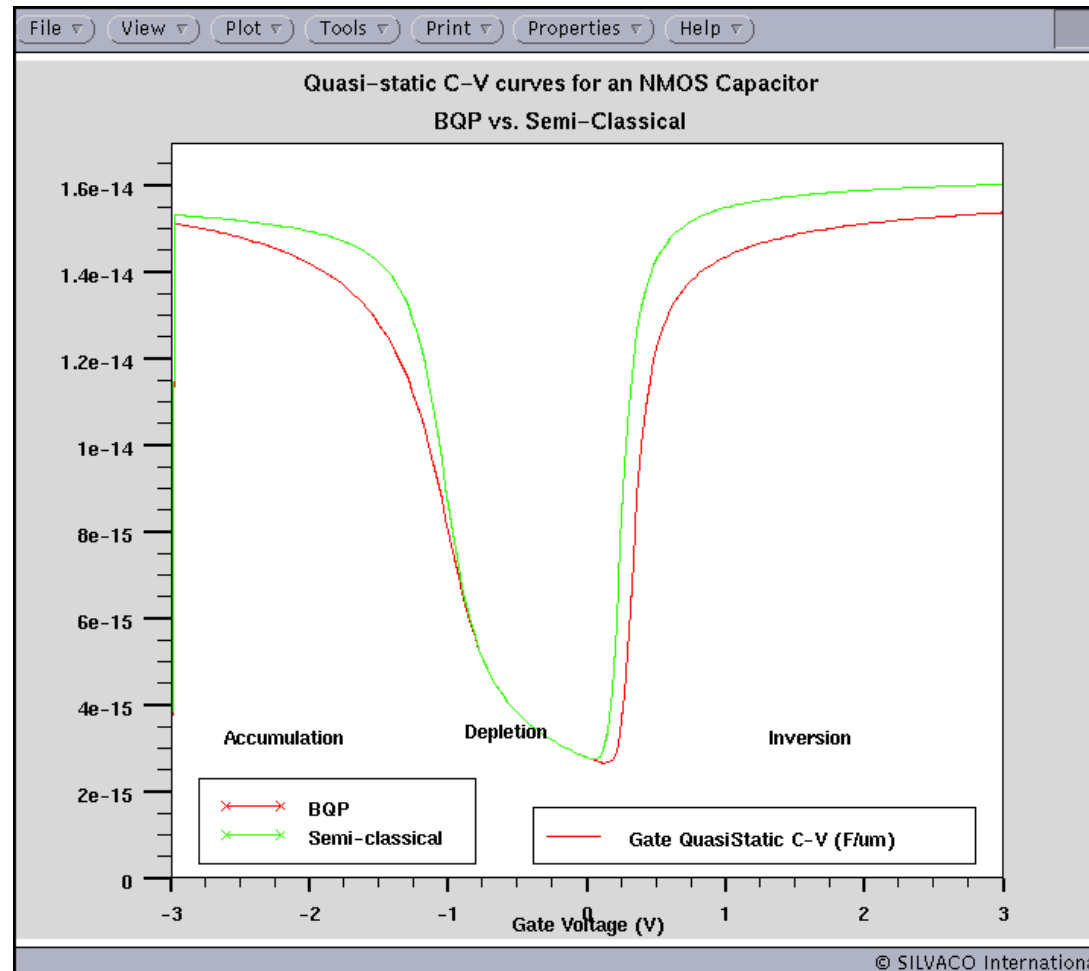


BQP Calibration to Schrodinger-Poisson





BQP Comparison with Classical



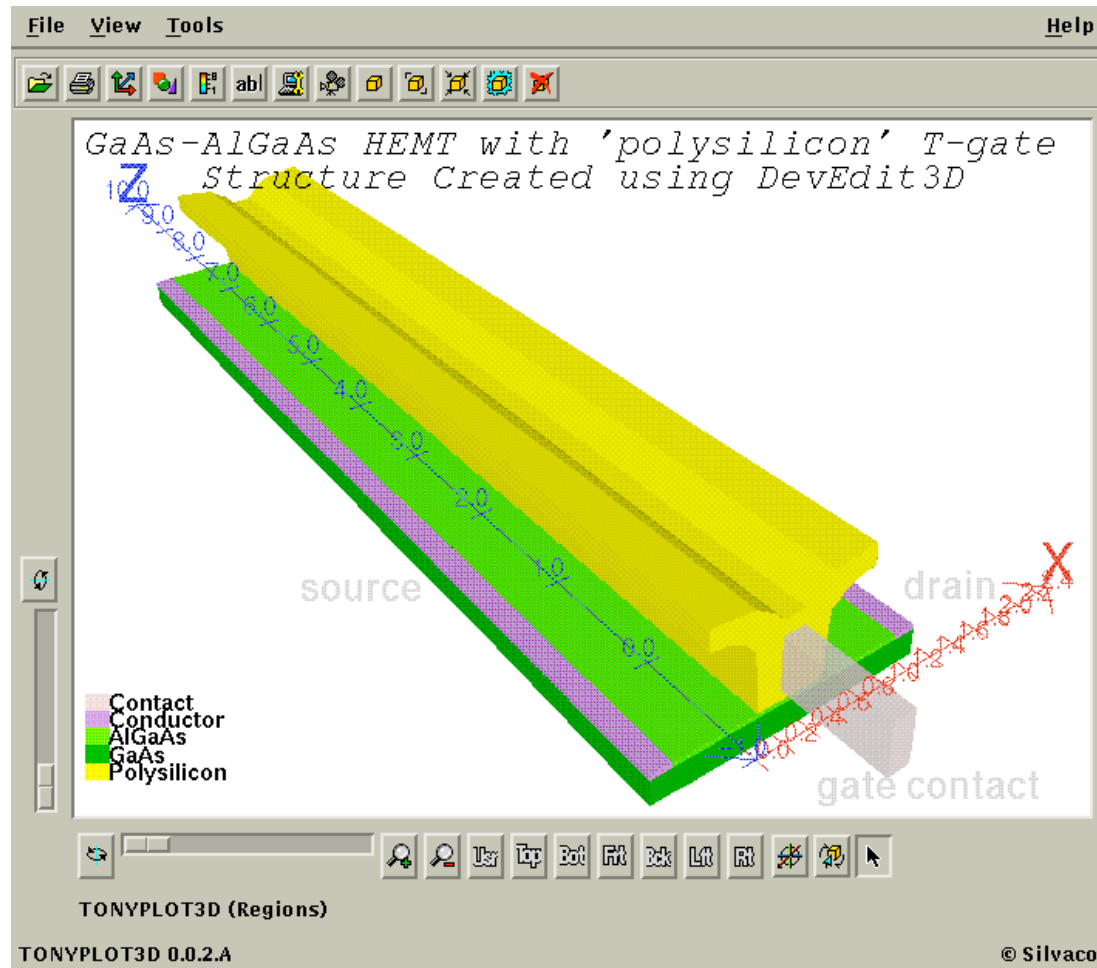


Quantum Effects in Optical Models

- Schrodinger solutions for bound state energies
- Bound state energies used in gain, spontaneous recombination and absorption models to predict allowed transitions



3D Hetrostructure Simulation





Quantum Correction Models I: Hansch Model

- Calculates confinement near gate oxide in MOSFET
- Correction factor modifies density of states
- Syntax: MODEL HANSCH

Reference: Hansch, W., Vogelsang, Th., Kirchner, R., and Orlowski, M.
“Carrier Transport Near the Si/SiO₂ Interface of a MOSFET”
Solid State Elec. Vol 32, no. 10 pp 839-849, 1989.



Quantum Correction Models II: Van Dort Model

- Intended for quantum confinement near Si/SiO₂ interfaces
- Confinement modeled by broadening of the bandgap near interface
- Syntax: MODEL N.DORT

Reference: Van Dort, M.J., Woerlee, P.H., and Walker, A.J. “ A Simple Model for Quantisation Effects in Heavily-Doped Silicon MOSFETs at Inversion Conditions” Solid State Elec., vol. 37, no 3, pp 411-414, 1994.



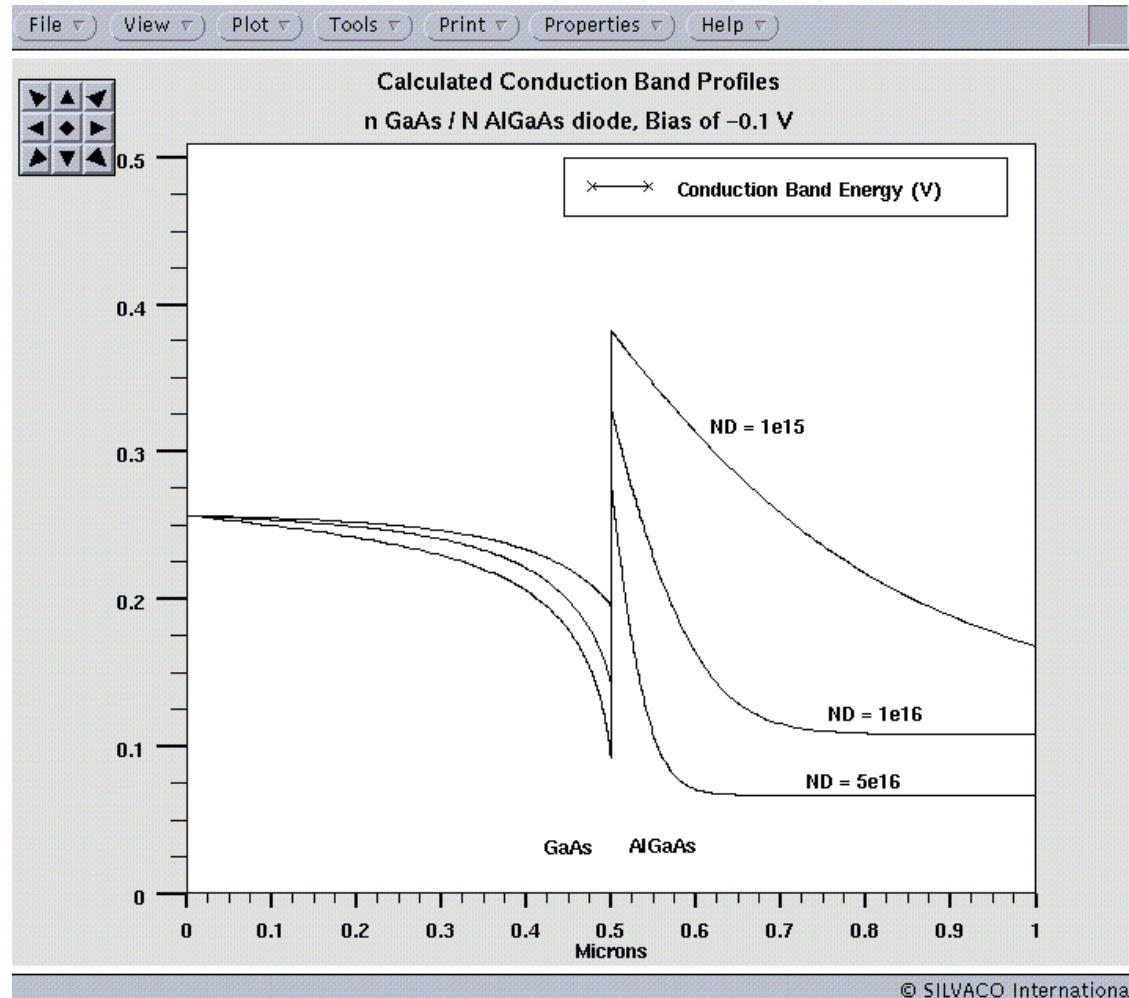
Thermionic Emission and Tunneling models I: Heterojunction

- Some Quantum Effects are included as physical models in BLAZE:
 - Thermionic-field emission boundary condition based on the WKB approximation
 - Thermionic emission and thermionic-field emission (tunneling) across heterointerfaces
 - Isotype and p-n junctions
 - Uniform and graded composition fraction
 - Syntax: `INTERFACE THERMIONIC X.MIN X.MAN Y.MIN Y.MAX //` for thermionic emission model
 - Syntax: `INTERFACE THERMIONIC TUNNEL X.MIN X.MAN Y.MIN Y.MAX //` for both thermionic emission and tunneling
 - Syntax: `INTERFACE` statement directly after `MESH`, `REGION` and `ELECTRODE` statements, and before statements `MODEL` and `MATERIAL`

Reference: Yang et al. Solid-State Electronics, vol 36, no. 3, pp321-330, 1993

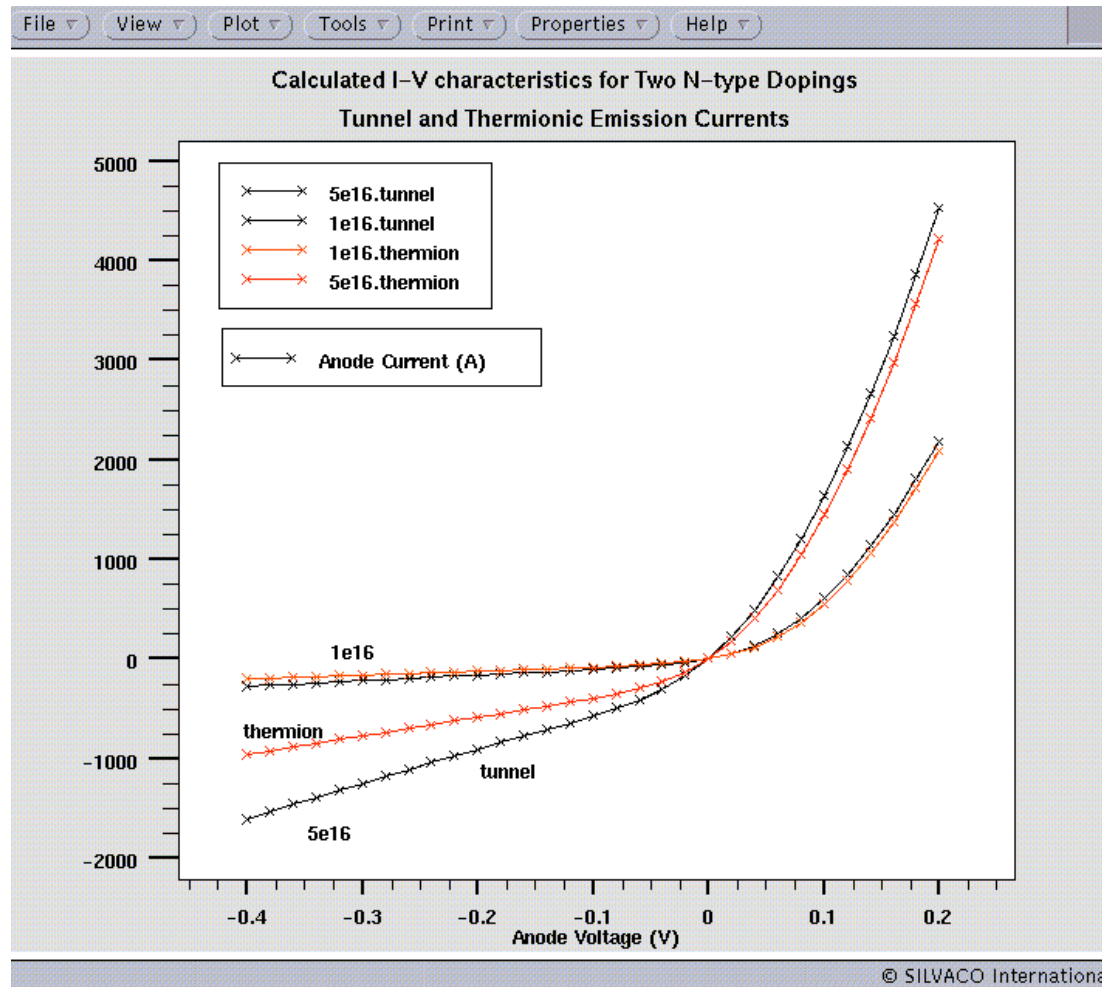


Thermionic Emission and Tunneling models I: Heterojunction





Thermionic Emission and Tunneling models I: Heterojunction





Thermionic Emission and Tunneling models II: Schottky Contact

- ATLAS: BLAZE
- Metal - semiconductor junction
- Models tunneling and thermionic emission at Schottky contacts
- Surface recombination enabled
- Syntax: CONTACTS E.TUNNEL



Conclusion

- Quantum models required for thin material layers (gate oxides, HEMTs, etc.)
- ATLAS provides variety of quantum models
 - Schrodinger-Poisson - solver for eigenstates
 - Quantum Moments gives carrier concentration and current
 - Specialized MOS correction models
- Some tunneling/emission effects modeled through separate models in BLAZE