Quantum Electronic Device Simulation

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March 10, 1997

Quantum Electronic Device Simulation

Outline

- Motivation
- Approach
- Transfer-Matrix Method
- Wigner Function Method
- Quantum Self-Consistency
- Transient Bias Slewing
- Resonant Tunneling Diode Physics
- Conclusions

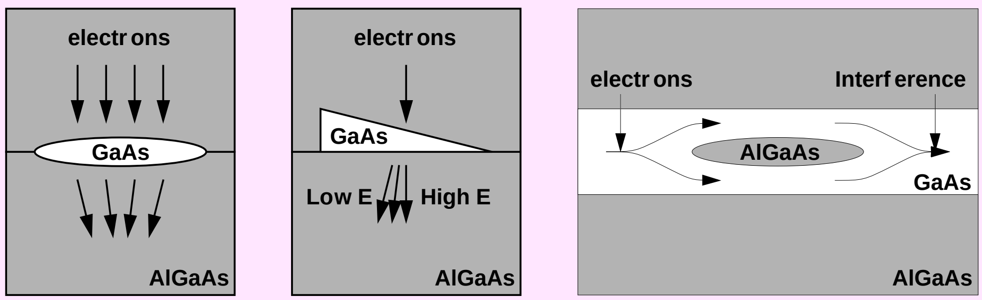
What is a Quantum Device?

Quantum scale: “particles” act like waves.

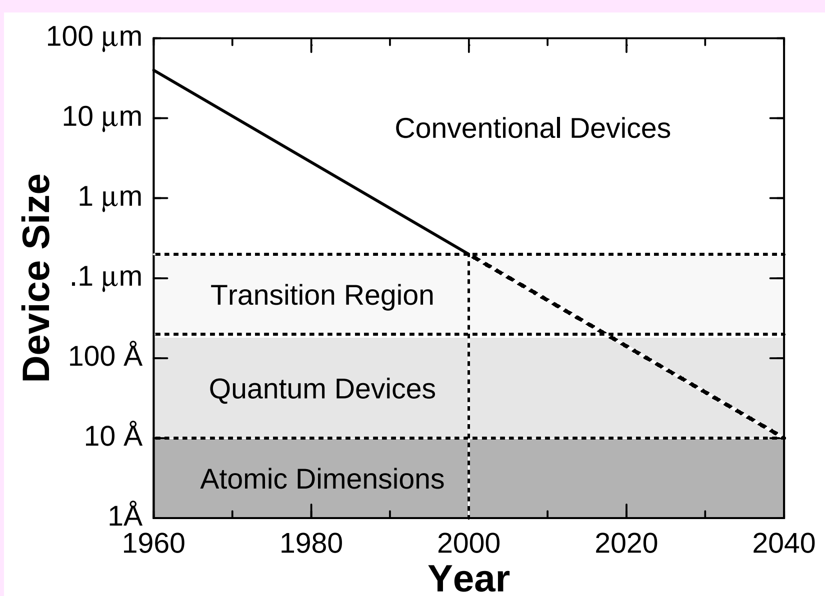
Quantum device: operation is based on quantum wave behavior of electrons.

Simple Quantum Devices

Electron Lens | **Electron Prism** | **Electron Interferometer**

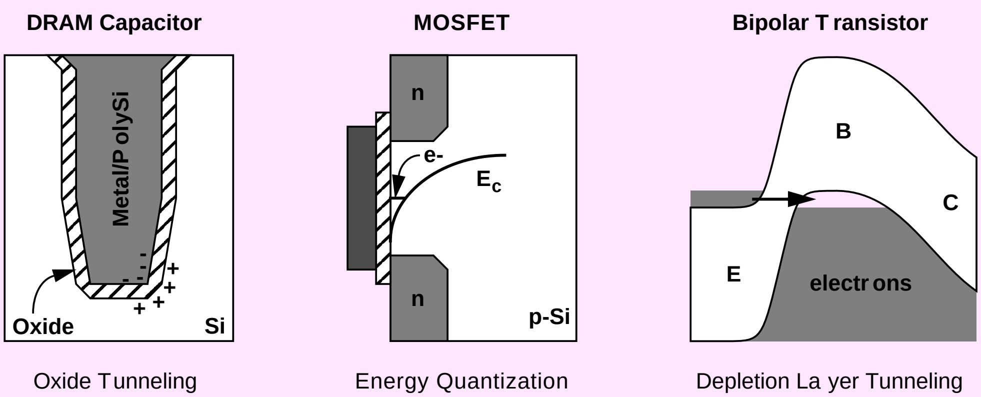


Future of Electronic Device Scaling

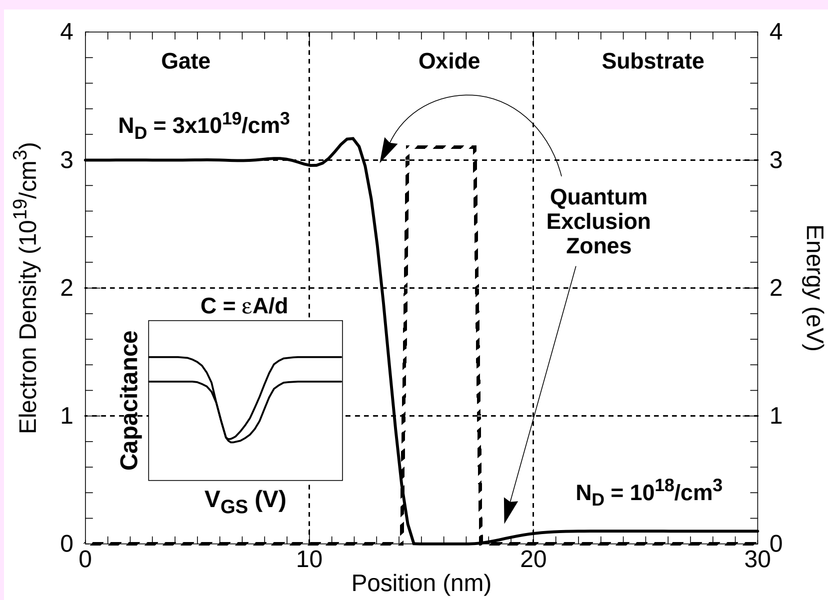


Quantum Effects in Conventional Devices

Quantum effects are an increasing “nuisance” in shrinking conventional electronic devices.



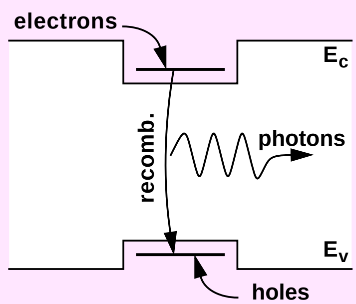
Quantum Effects in MOSFET



Hybrid Conventional-Quantum Devices

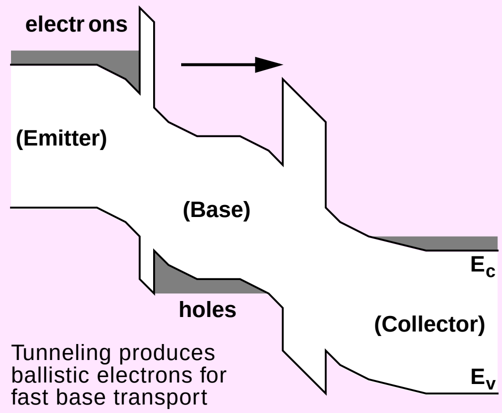
New heterojunction devices use quantum effects.

Quantum Well Laser Diode



Quantum well confines carriers
for more controlled recombination

Hot Electron Transistor

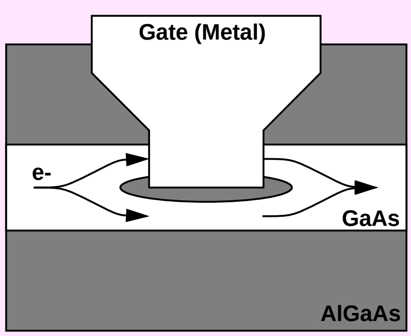


Tunneling produces
ballistic electrons for
fast base transport

Quantum Electronic Devices

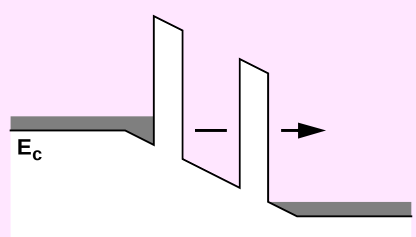
True quantum devices promise much further down-scaling.

Quantum Interference Transistor

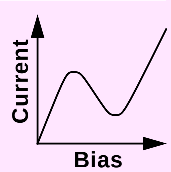


Gate bias modulates electron
wavelength and resulting interf erence

Resonant T unneling Diode



Resonant energy
level in quantum well
produces negativ e
differential resistance



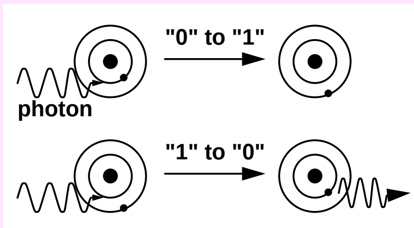
Why Investigate Quantum Devices? (4)

Quantum computers may solve otherwise "impossible" problems:

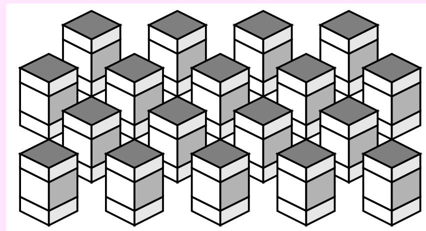
- Quantum decryption
- Provably secure communication
- Real-time simulation of quantum systems

Ultimate Quantum Systems

Possible Quantum Device: Hydrogen Atom



Possib le Quantum Computer: Quantum Dot Arra y



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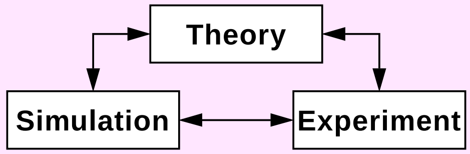
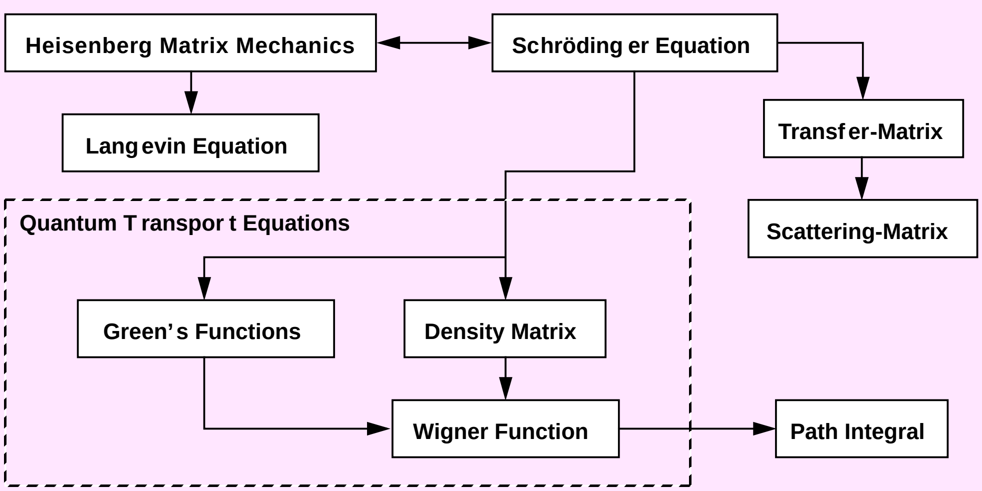
Goals of Quantum Device Simulation



Strengths of simulation:

- More detail than theory
- Internal view of device operation
- Modify device and test conditions at will
- Vastly less expensive than experiment

Formulations of Quantum Mechanics



Approaches in SQUADS (to efficiently simulate real quantum systems):

- Wigner function method
- Transfer-matrix method

Guiding Principles for SQUADS

(Stanford QUAntum Device Simulator)

- General (any 1-D structure and material system)
- Comprehensive test suite (steady-state, transient, small-signal)
- Designed for investigation of quantum device *simulation*:
  - Structural modularity
  - Comparison of efficiency, accuracy, and robustness
- Computationally efficient (CPU and memory)
- Automated (minimal user effort)

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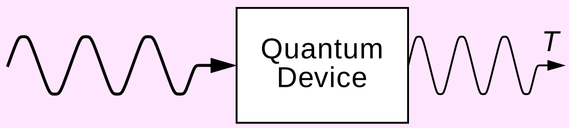
Overview of Transfer-Matrix Method (TMM)

Premise: Determine current flow from transmission *T* of a beam of particles through device.

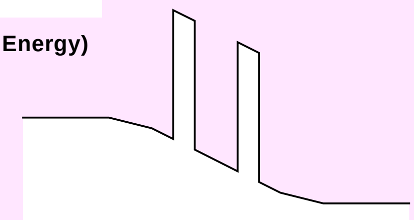


Calculate *T* from time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + U(x)\psi(x) = E\psi(x)$$

(Kinetic + Potential = Total Energy)

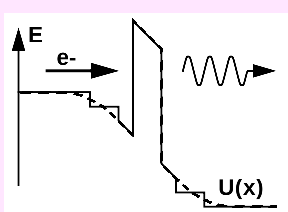
But Schrödinger equation can't be solved analytically for *U(x)* in useful quantum devices.



Resonant Tunneling Diode

Solving the Schrödinger Equation

TMM Approach: Divide device into many short regions.
Approximate U(x) as "solvable" function in each region.



$$E > U_1(x) = c_1 \Rightarrow \psi(x) = a_1 e^{ik_1 x} + b_1 e^{-ik_1 x}$$

$$E < U_2(x) = c_2 \Rightarrow \psi(x) = a_2 e^{\kappa_2 x} + b_2 e^{-\kappa_2 x}$$

$$U_3(x) = c_3 + d_3 x \Rightarrow \psi(x) = a_3 \mathrm{Ai}(z) + b_3 \mathrm{Bi}(z)$$

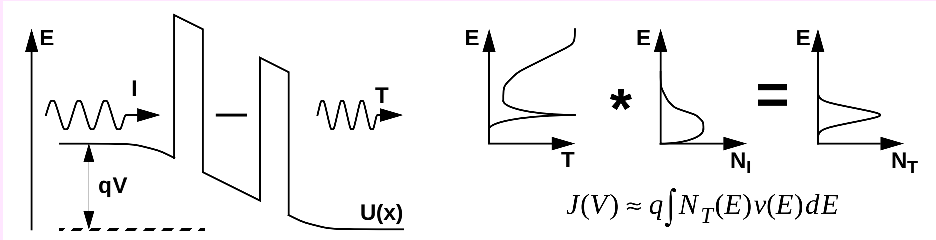
But now there are two unknowns for each region!

Wavefunction matching conditions give enough constraints:

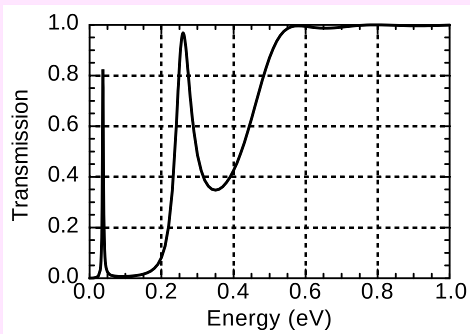
$$\psi_1(x) = \psi_2(x), \qquad \left.\frac{1}{m_1}\frac{\partial\psi_1}{\partial x}\right|_{x_1} = \left.\frac{1}{m_2}\frac{\partial\psi_2}{\partial x}\right|_{x_1}$$

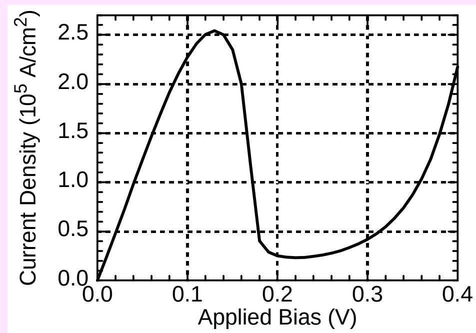
$$\begin{aligned} a_2 &= t_{11}a_1 + t_{12}b_1 \\ b_2 &= t_{21}a_1 + t_{22}b_1 \end{aligned}, \qquad \begin{bmatrix} a_2 \\ b_2 \end{bmatrix} = \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix}\begin{bmatrix} a_1 \\ b_1 \end{bmatrix}, \qquad \begin{bmatrix} T \\ 0 \end{bmatrix} = \begin{bmatrix} t_N \end{bmatrix}\begin{bmatrix} t_{N\text{-}1} \end{bmatrix}\cdots\begin{bmatrix} t_1 \end{bmatrix}\begin{bmatrix} t_0 \end{bmatrix}\begin{bmatrix} I \\ R \end{bmatrix}$$

TMM Simulation Procedures and Results



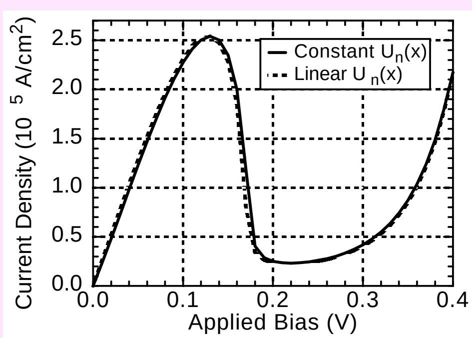
$$J(V) \approx q\int N_T(E)v(E)dE$$





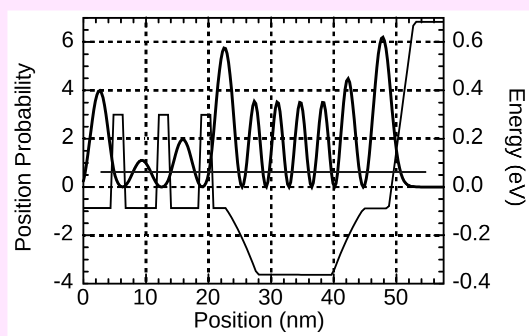
TMM Simulation: Beyond the Basics

Constant versus Linear Potential Regions



Linear regions not w orth the eff ort

Wavefunction Calculation



Material model parameter s:

- energ y band names
- band offsets
- eff ective mass
- permittivity
- strain dependence

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Wigner Function Method (WFM)

Analogous to the Boltzmann transport equation (BTE) formulation of classical physics:

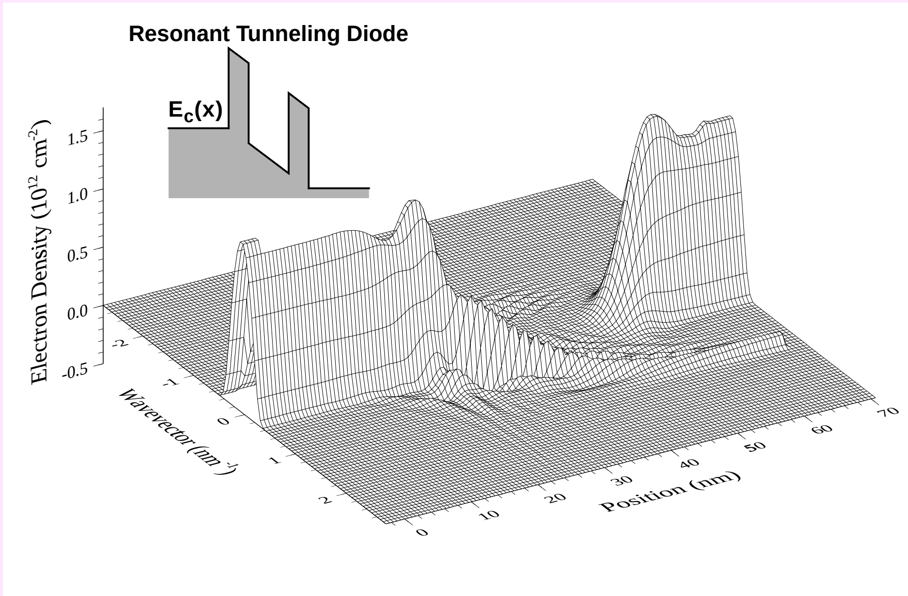
$$\frac{\partial f_c}{\partial t} = -\underbrace{\vec{v}\frac{\partial f_c}{\partial \vec{r}}}_{\text{diffusion}} - \underbrace{\frac{\vec{F}}{\hbar}\frac{\partial f_c}{\partial \vec{k}}}_{\text{drift}} + \underbrace{\left[\frac{\partial f_c}{\partial t}\right]_{\text{coll}}}_{\text{scatering}}$$

Wigner Function transport equation (WFTE) in 1-D:

$$\frac{\partial f_w}{\partial t} = -\underbrace{\frac{\hbar k}{m}\frac{\partial f_w}{\partial x}}_{\text{diffusion}} - \underbrace{\frac{1}{\hbar}\int\frac{dk'}{2\pi}V(x, k-k')\,f_w(x, k')}_{\text{drift}} + \underbrace{\left[\frac{\partial f_w}{\partial t}\right]_{\text{coll}}}_{\text{scatering}}$$

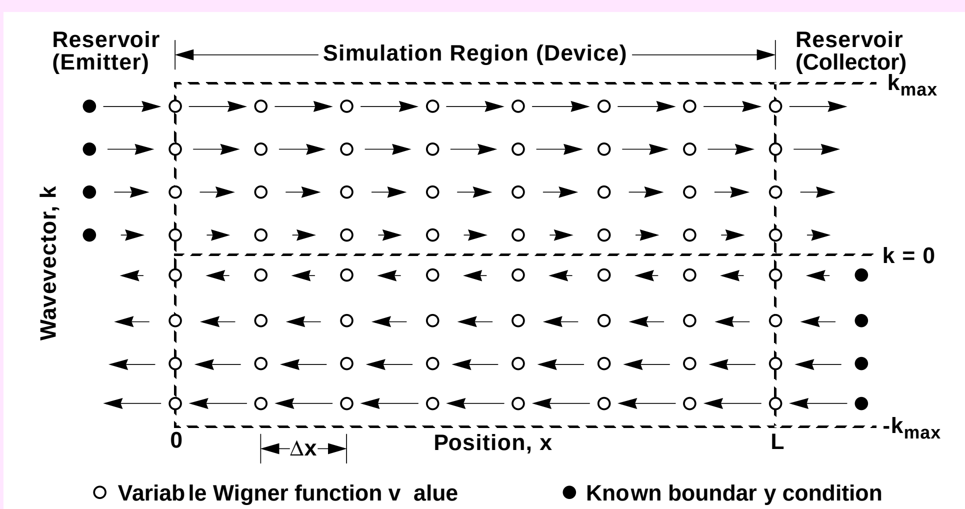
State functions like f_c and f_w are natural, efficient, and intuitive.

RTD Wigner Function at High Bias



Wigner Function Gridding Scheme

For numerical solution of WFTE, approximate Wigner function as array of values at discrete (x,k) pairs.



WFTE Discretization

Write each term in WFTE in terms of the discrete WF values

$$\frac{\partial f_w}{\partial t} = -\underbrace{\frac{\hbar k}{m}\frac{\partial f_w}{\partial x}}_{\text{diffusion}} - \underbrace{\frac{1}{\hbar}\int\frac{dk'}{2\pi}V(x, k-k')\,f_w(x, k')}_{\text{drift}} + \underbrace{\left[\frac{\partial f_w}{\partial t}\right]_{\text{coll}}}_{\text{scatering}}$$

Examples: First-order transient term and first-order upwind difference diffusion term:

$$\frac{\partial f_w}{\partial t} \approx \frac{f(x_i, k_j, t_{n+1}) - f(x_i, k_j, t_n)}{\Delta t}$$

$$\left[\frac{\hbar k}{m}\frac{\partial f_w}{\partial x}\right]_{x_i} \approx \frac{\hbar k_j}{m\Delta x}\left\{\begin{matrix} f(x_{i+1}, k_j) - f(x_i, k_j) & (k_j < 0) \\ f(x_i, k_j) - f(x_{i-1}, k_j) & (k_j > 0) \end{matrix}\right\}$$

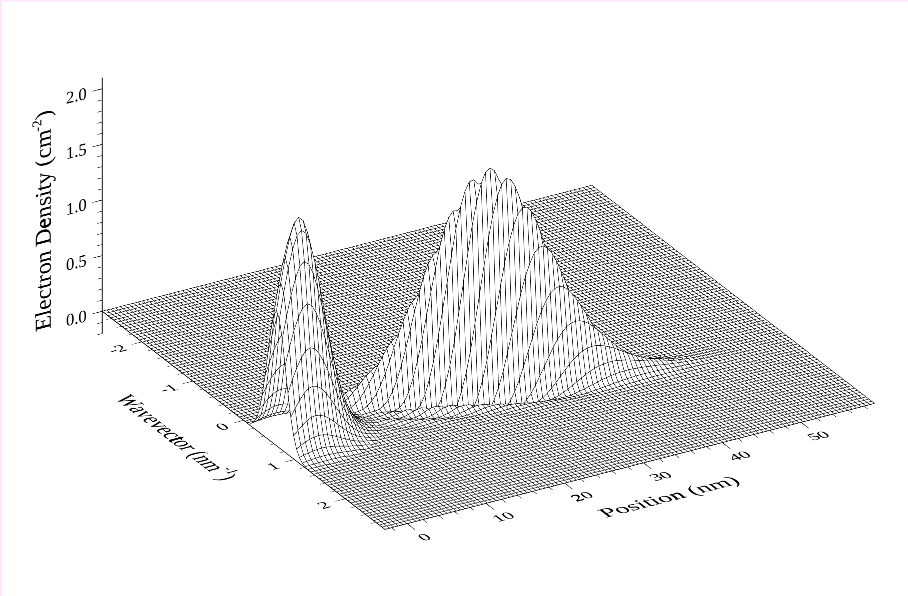
WFTE Discretization Options

Alternate discretization schemes implemented in SQUADS:

- Transient term: 1st and 2nd order forward and backward Euler, Cayley.
- Diffusion term: 1st, 2nd, and 3rd order upwind; 2nd, 4th, and 6th order central; any hybrid combination; simple m*(x) model.
- Drift term integration methods: Standard, rectangular-smoothed, triangular-smoothed.
- Scattering term: Relaxation-time approximation.

Trade-off: efficiency versus accuracy

Gaussian Wave Packet: 20 fs Simulation



WFTE Discretization Conclusions

Transient term:

- FE1, FE2, BE2 can diverge
- Cayley more accurate than BE1

Diffusion term:

- High order forms (UDS3, CDS6) unnecessary
- Hybrid difference schemes (e.g., UDS2/CDS2) optimal
- Changing difference scheme at boundary (HDS, CDS) acceptable
- Simple m*(x) model: high error

Drift term: Alternative forms add little error.

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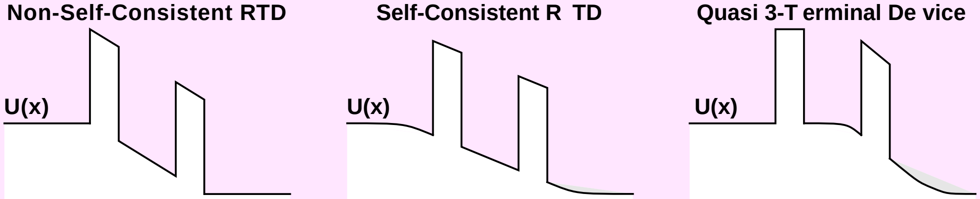
What is Self-Consistency?

Self-Consistency: Carrier density profile c(x) is consistent with the energy band profile U(x), as dictated by the Poisson equation (PE)

WFTE-PE system is a non-linear pair of equations:

- PE: $\frac{\partial}{\partial x}\left[\varepsilon(x)\frac{\partial}{\partial x}u(x)\right] = q\rho(x) = q^2[C(x) - c(x)], \quad u(x) = U(x) - \delta U(x)$
- WFTE: $\frac{\partial f_w}{\partial t} = -\underbrace{\frac{\hbar k}{m}\frac{\partial f_w}{\partial x}}_{\text{diffusion}} - \underbrace{\frac{1}{\hbar}\int\frac{dk'}{2\pi}V(x, k-k')\, f_w(x, k')}_{\text{drift}} + \underbrace{\left[\frac{\partial f_w}{\partial t}\right]_{\text{coll}}}_{\text{scatering}}$

Non-Self-Consistent RTD **Self-Consistent R TD** **Quasi 3-T erminal De vice**



Poisson Equation in SQUADS

Self-consistent solution of WFTE-PE system requires iteration.

Differential form of PE used in SQUADS: includes feedback term.

Expressions for dc/dU feedback term:

Classical M-B: $c(u) = N_c \exp[(u - u_0)/k_B T]$, $\quad \frac{\partial c}{\partial u} = \frac{c(u)}{k_B T}$

Classical F-D: $\frac{\partial c}{\partial u} = \frac{N_c}{k_B T}\left[\frac{1}{R} + \sum_{m=1} \frac{a_m}{m} R^{m-1}\right]^{-1}, \quad R \equiv \frac{c}{N_c}$

Quantum: Full Newton form (described for first time)

Self-Consistency Iteration Approaches

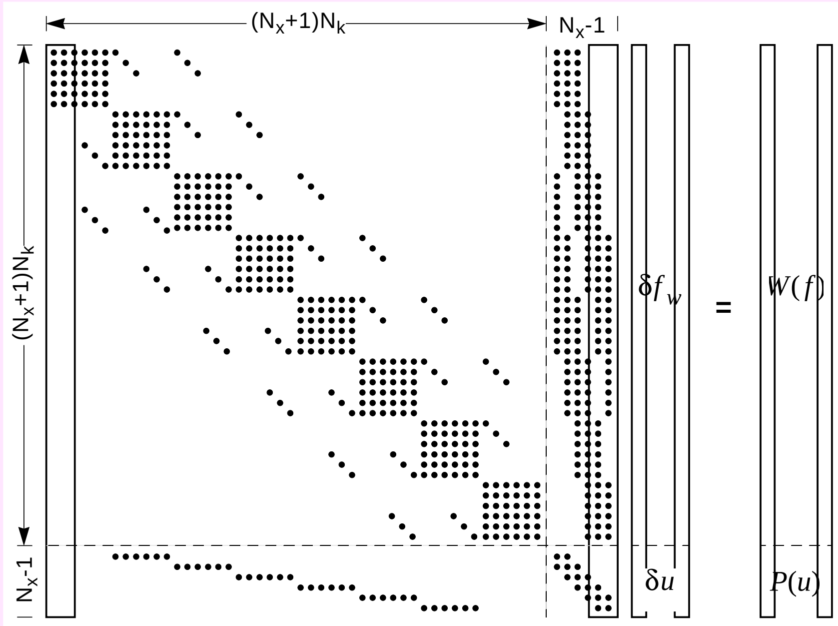
SQUADS implements two general approaches for N-L system iteration:

- Gummel (plug-in): Solve equations consecutively with approximate feedback term. Low computational cost.
- Newton: Solve single system of all equations with exact feedback. Fewer iterations, but high cost per iteration.

Two solution modes for each:

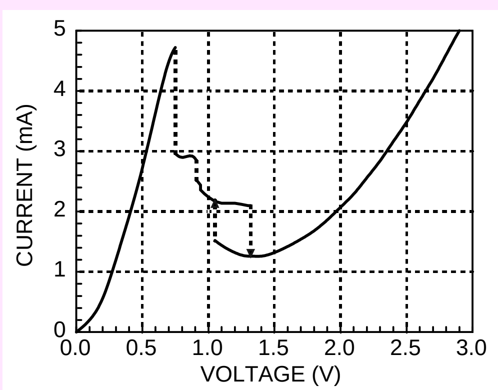
- Steady-state: Find self-consistent solution ASAP. Intermediate solutions are meaningless.
- Transient: Each S-C iteration is also a time step. Intermediate solutions follow evolution of device.

Full-Newton WFTE-PE Matrix Equation

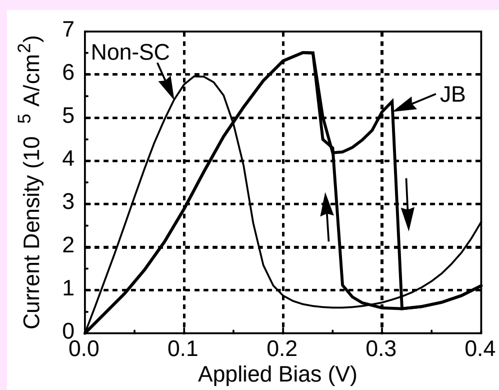


Test Device Expected Results

Experimental RTD I-V Curve
(Brown et al., APL 55, 1777)

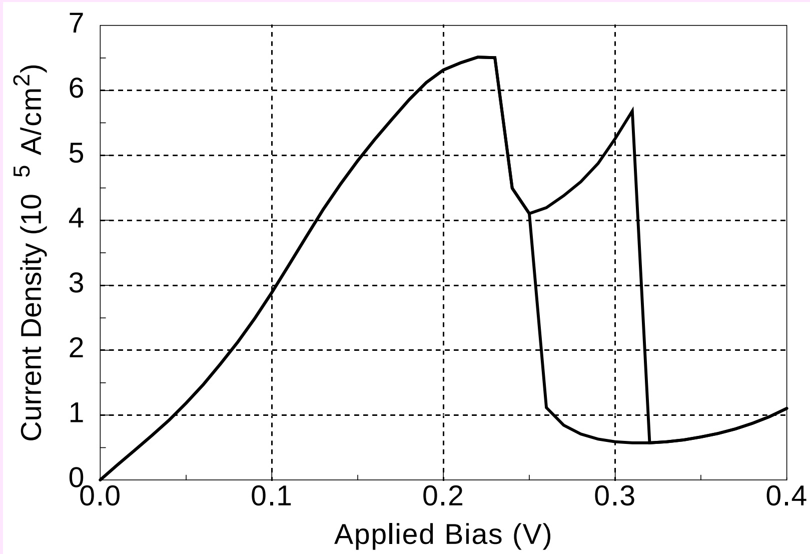


WFM Simulated RTD I-V Curve
(Jensen and Buot, PRL 66, 1078)



JB simulations first to reproduce experimental RTD behavior in NDR region: I-V plateau, hysteresis, bistability, and unstable oscillations.

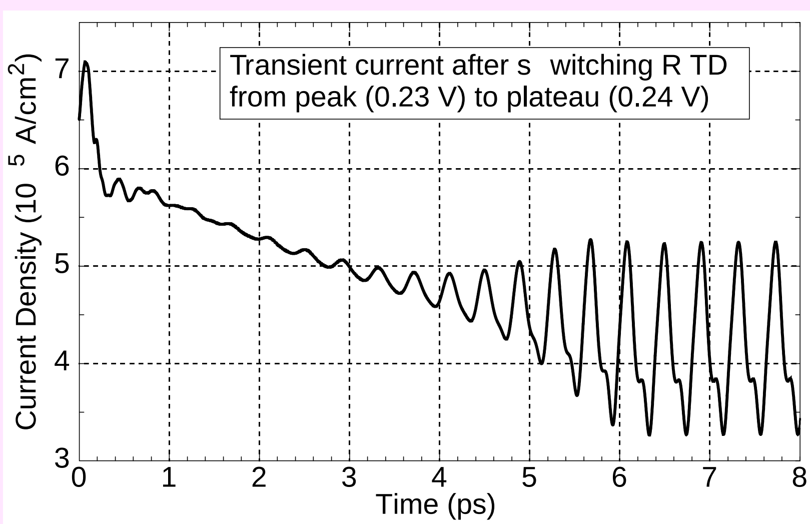
Steady-State Self-Consistency Results



Conclusion: Plateau is not a purely transient effect, as in experiment!

SELF-CONSISTENCY

Transient Self-Consistency Results



RTD is unstable in NDR portion of plateau.
Steady-state simulations gave no clue!

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Self-Consistency Conclusions

Performance Results

Self-Consistency Iteration Method	CPU Hour s
Steady-State Gummel (M-B)	14.3
Steady-State Gummel (F-D)	5.0
Steady-State Ne wton	7.2
Transient Gummel	330
Transient Ne wton	~1,650

- Both steady-state and transient iterations required for max utility.
  - Steady-state for efficient, wide-ranging investigations.
  - Transient for ultimate accuracy and transient situations.
- SS Gummel with F-D feedback improves CPU time by factor of 3.
- Newton method not worth computational price (2xRAM, 1.5xCPU).
- SS Gummel with M-B feedback needed where convergence difficult.

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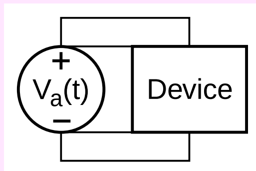
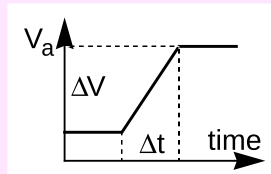
Conventional Bias Slewing Approach

Applied bias slew rate: rate of change of applied bias with time.





SR = ΔV/Δt

Standard quantum simulation approach: “instantaneous” bias changes

For typical quantum device simulation, time step is 1 fs ($1e^{-15}$ s)!

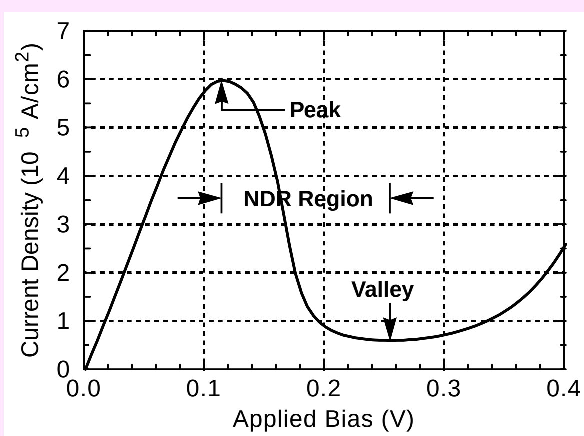
Problem: resulting slew rate for I-V curve trace is 10 V/ps!

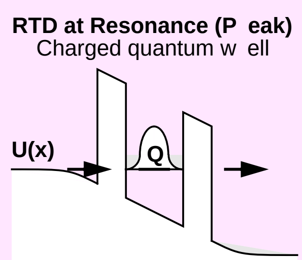
But fast operational amplifiers can produce only 1-10 V/ns.

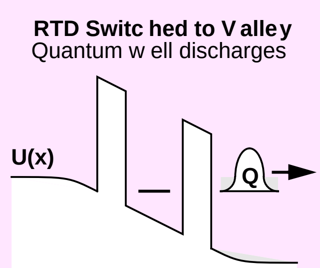
Conclusion: standard bias switching approach in quantum simulation is unrealistic, but does it matter?

Bias Change Current Pulse (1)

Most transient simulations involve switching across the NDR region.

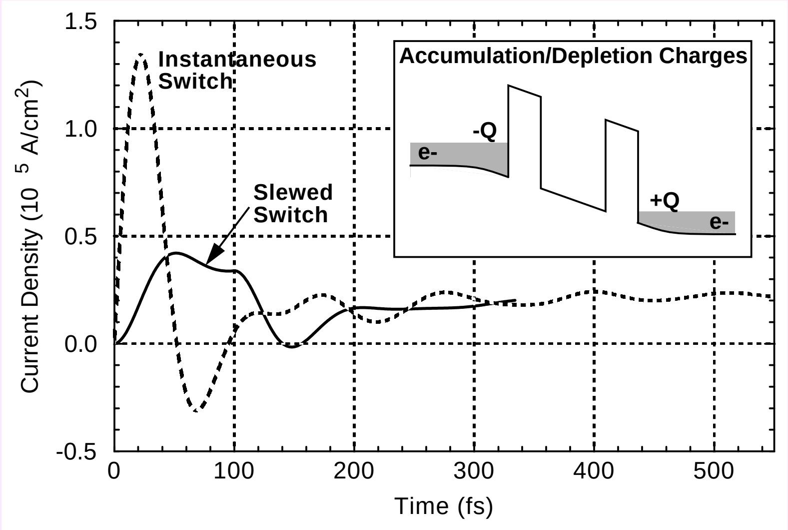






Current pulse after switching was assumed to be due to quantum well (dis)charging.

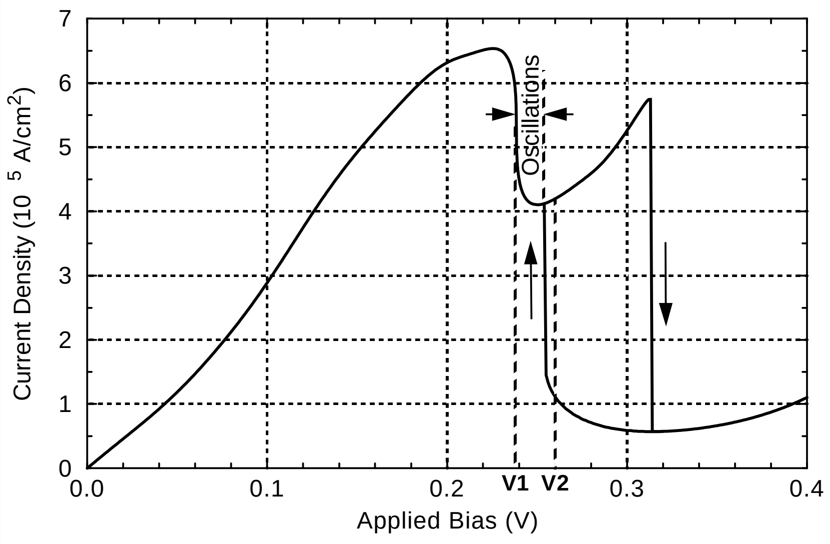
Bias Change Current Pulse (2)



Current pulse is usually due to accumulation/depletion charging.

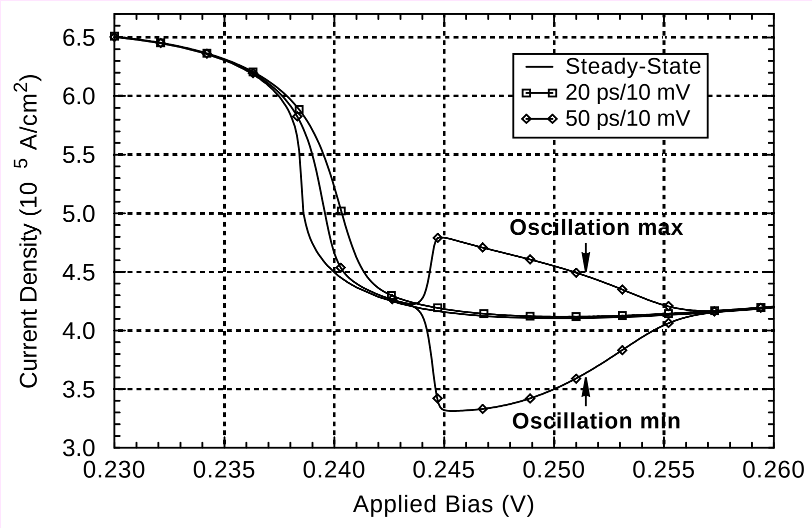
Instantaneous switching causes more severe transient response.

Review: Steady-State RTD I-V Curve



Note oscillation region between V1 and V2, and bistable operation at V2.

Slewing Through Critical Regions

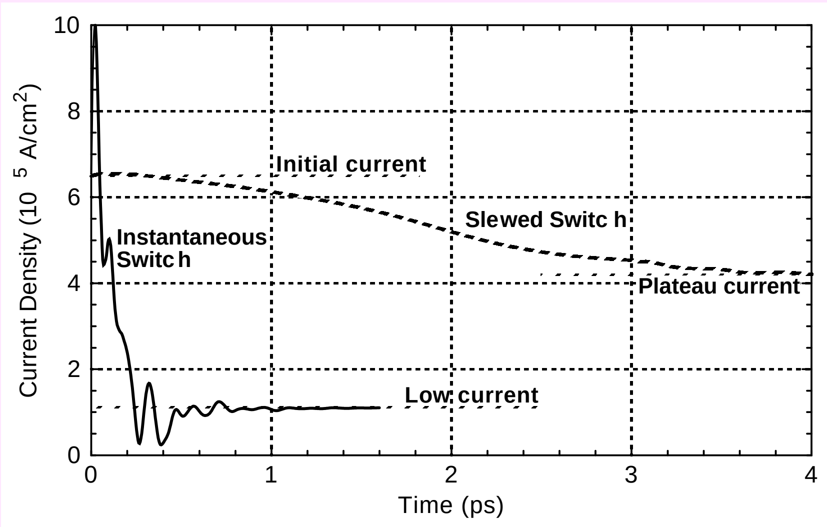


Observation: Some processes in RTD are (relatively) very slow.

Conclusion: Low slew rate is sometime required.

SLEW RATE

Slewing into Bistable Regions



Observation: Device function depends on slew rate.

Conclusion: Simulated slew rate should mirror intended application.

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Slew Rate Investigation Conclusions

Applied bias slew rate does affect quantum device function:

- Huge current pulses due to instantaneous switching
- Slewing too quickly across critical regions
- Slewing into a bistable region

Some processes in RTDs are unexpectedly slow.

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Open RTD Questions/Controversies

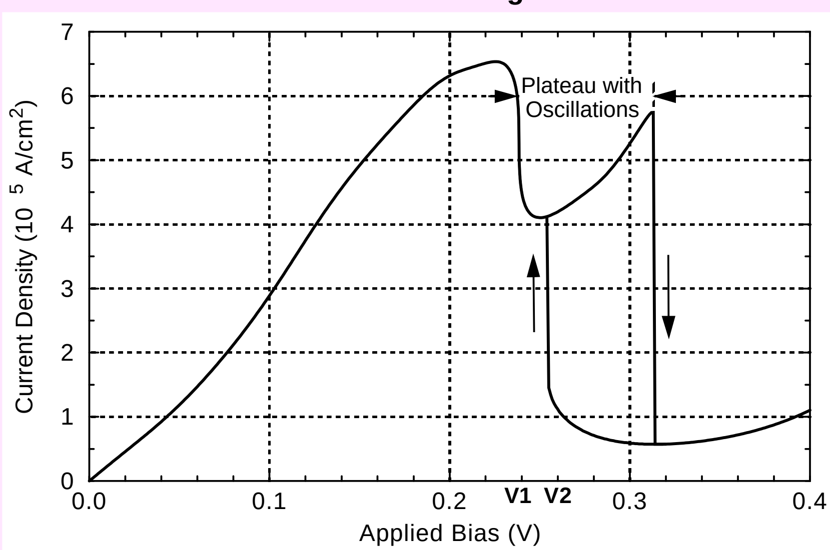
- Cause of observed I-V plateau and associated oscillations
- Existence and appearance of intrinsic bistability
- Correct lumped-parameter equivalent circuit model

WFM simulations of Jensen and Buot contradicted the consensus view on each of these issues.

SQUADS was used to investigate, with surprising results....

Review of Jensen and Buot Results

JB RTD Current-Voltage Curve

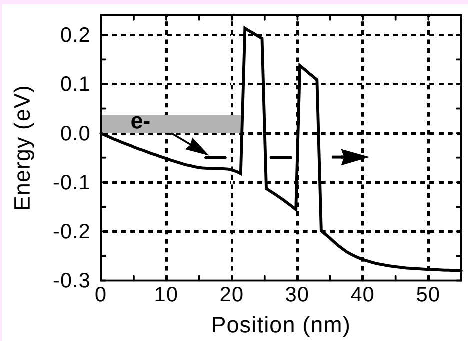


Cause of I-V Plateau and Oscillations

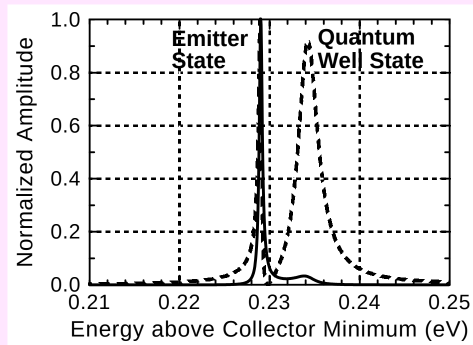
Consensus: observed I-V plateau is average of high-frequency oscillations, requiring external inductance.

SQUADS (and JB) simulations produced purely intrinsic plateau.

Energy Band Profile in Plateau

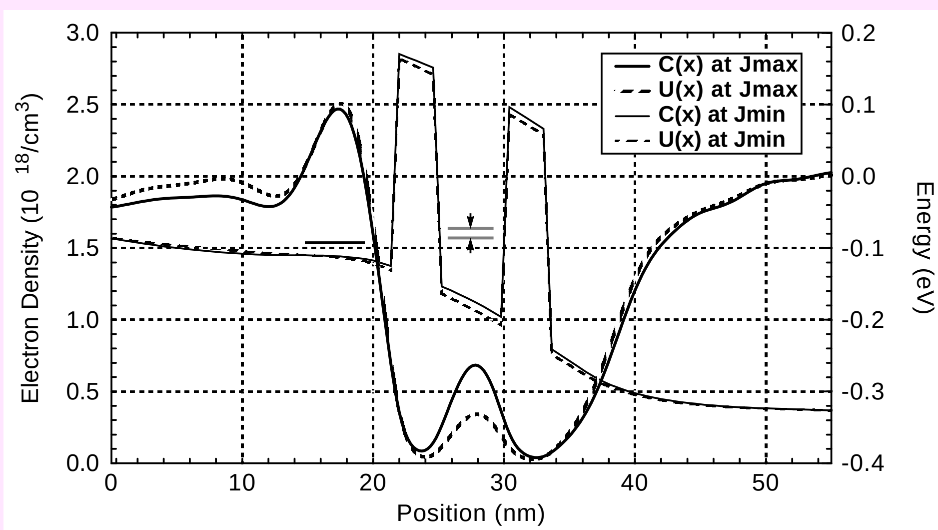


Quantized Energy Levels in Plateau



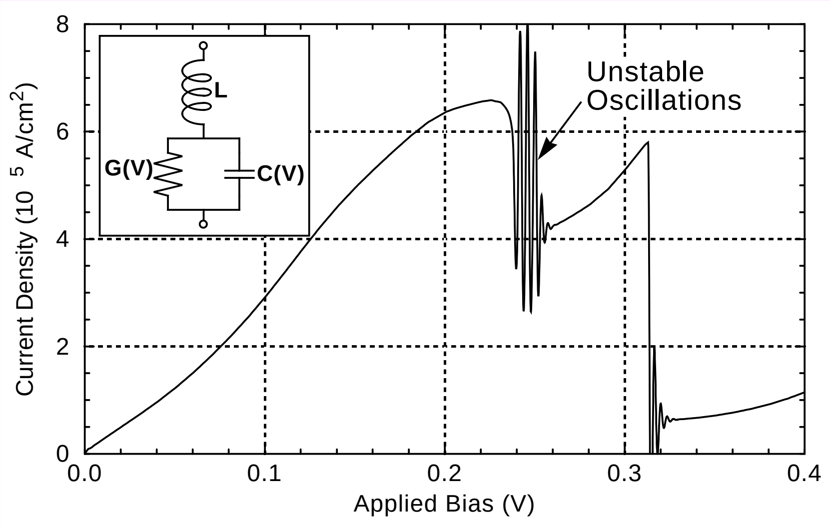
Conclusion: Simulated I-V plateau due to a new steady-state current path, not oscillations.

Cause of Simulated Oscillations



Oscillations due to alternating charge in emitter and QW, and resulting variation in alignment of discrete states.

RTD Equivalent Circuit Model



Simulated I-V curve completely explained by conventional circuit model. JB parallel inductance model too unstable.

Contradiction: Simulation vs Experiment

Simulation results above still disagree with experiment on key points:

- Simulated plateau is steady-state effect.
- Simulated plateau only unstable in small region.
- Simulated steady-state bistability appears in plateau.

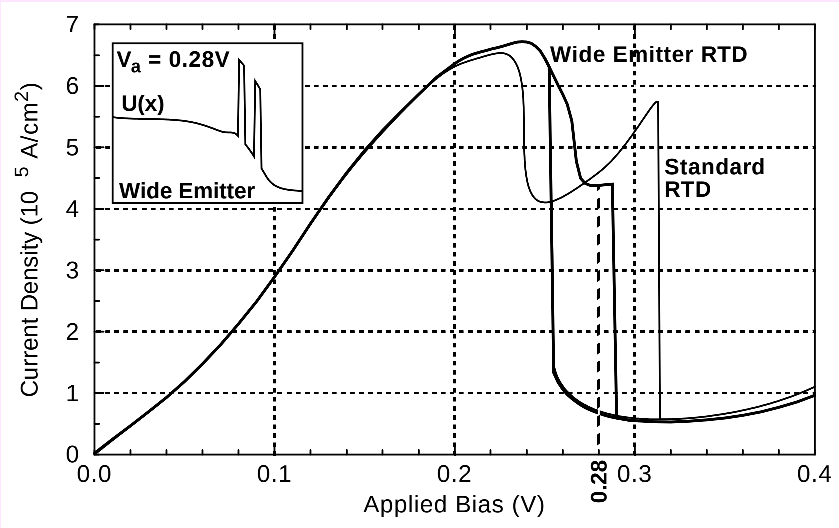
But device doesn't match experiment either:

- Simulated device not charge-neutral: charged contacts.
- Potential depression in emitter not seen in experiment.

JB's conclusions not supported:

- that they had reproduced experimental observations
- that consensus on some RTD controversies should be revised

Wide Emitter RTD I-V Curve



Simulated plateau much smaller. Bistability in main peak now closer to experimental results.

RTD Physics Investigation Conclusions

Most detailed simulation investigation of RTD operation to date:

- Uncovered and corrected errors in previous investigations of simulation results and experiment.
- Achieved improved agreement between simulation and experiment for the RTD.

Quantum Electronic Device Simulation

Outline

- Motivation
- Approach
- Transfer-Matrix Method
- Wigner Function Method
- Quantum Self-Consistency
- Transient Bias Slewing
- Resonant Tunneling Diode Physics
- **Conclusions**

Contributions

- SQUADS: a highly functional, efficient, and extensible simulation tool for simulation of 1-D quantum devices
- Advancements in Wigner function method:
  - Optimal discretization approaches determined
  - Complementary roles of steady-state and transient self-consistency iteration
- Detailed simulation investigation of RTD:
  - Applied bias slew rate can dramatically change device function
  - Corrected errors in previous interpretation of simulation and experiment
  - Improved agreement between simulation and experiment

Publications

B. A. Biegel and J. D. Plummer, “Comparison of self-consistency iteration options for the Wigner function method of quantum device simulation”, *Physical Review B*, **54**(11), 8070 (9/15/96).

B. A. Biegel and J. D. Plummer, “Applied Bias Slewing in Transient Wigner Function Simulation of Resonant Tunneling Diodes”, *IEEE Transactions on Electron Devices*, **44**(5) (5/97).

B. A. Biegel and J. D. Plummer, “Simulation investigation of the physics of resonant tunneling diode operation”, (in preparation).

B. A. Biegel, *Quantum Electronic Device Simulation*, Ph.D. thesis, Stanford University, March 1997.