Numerical Algorithms Developed for Carrier Transport in Nanoelectronic Devices: Recursive Green Functions, NEGF, and Multiple Sequential Scattering

Quantitative simulations of carrier transport in physical systems that are of the size of a few nanometers require the use of quantum mechanical models at a very fundamental level. The non-equilibrium Green Function formalism provides a theoretical and practical framework that ties basic quantum mechanics with particle-particle interactions to electron transport through nano-scale structures. Basic algorithm approaches developed originally at Texas Instruments in the development of the nanoelectronic modeling tool (NEMO 1-D). Their utility for the modeling of electron and hole transport through resonant tunneling diodes will be presented. NEMO 1-D addresses the modeling needs for devices that have spatial variations in one dimension and where carrier transport crosses these interfaces. A glimpse of the recent NEMO–3D developments and an outlook on the challenges in the area of 3-D nanoelectronic modeling will conclude the presentation.

Dr. Gerhard Klimeck is the technical group supervisor of the Applied Cluster Computing Technologies Group and a Principal member at the NASA Jet Propulsion Laboratory. He joined JPL in February 1998 to engage in research in electron transport through nanoelectronic devices, parallel cluster computing, genetic algorithms, and parallel image processing. At JPL he has utilized technology in these areas to explore the nanoelectronic design space and has developed the 3-D Nanoelectronic Modeling tool (NEMO 3-D) that enables the analysis of electronic structure in systems containing as many as 32 million atoms. His work on mars image processing enabled near real-time data processing. Previously he was a member of technical staff at the Central Research Lab of Texas Instruments (which transitioned to the Applied Research Laboratory of Raytheon) where he served as manager and principal architect of the Nanoelectronic Modeling (NEMO) program. Dr. Klimeck received his Ph.D. in 1994 from Purdue University and Dipl. Ing from Ruhr-University Bochum, Germany. Dr. Klimeck's work is documented in over 75 peer-reviewed publications and over 120 conference presentations. Other authors have cited these publications over 300 times. He is a member of IEEE, APS, HKN and TBP.

http://hpc.jpl.nasa.gov/PEP/gekco provides more information about this research work.

Numerical Algorithms Developed for Carrier Transport in Nanoelectronic Devices: Recursive Green Functions, NEGF, and Multiple Sequential Scattering

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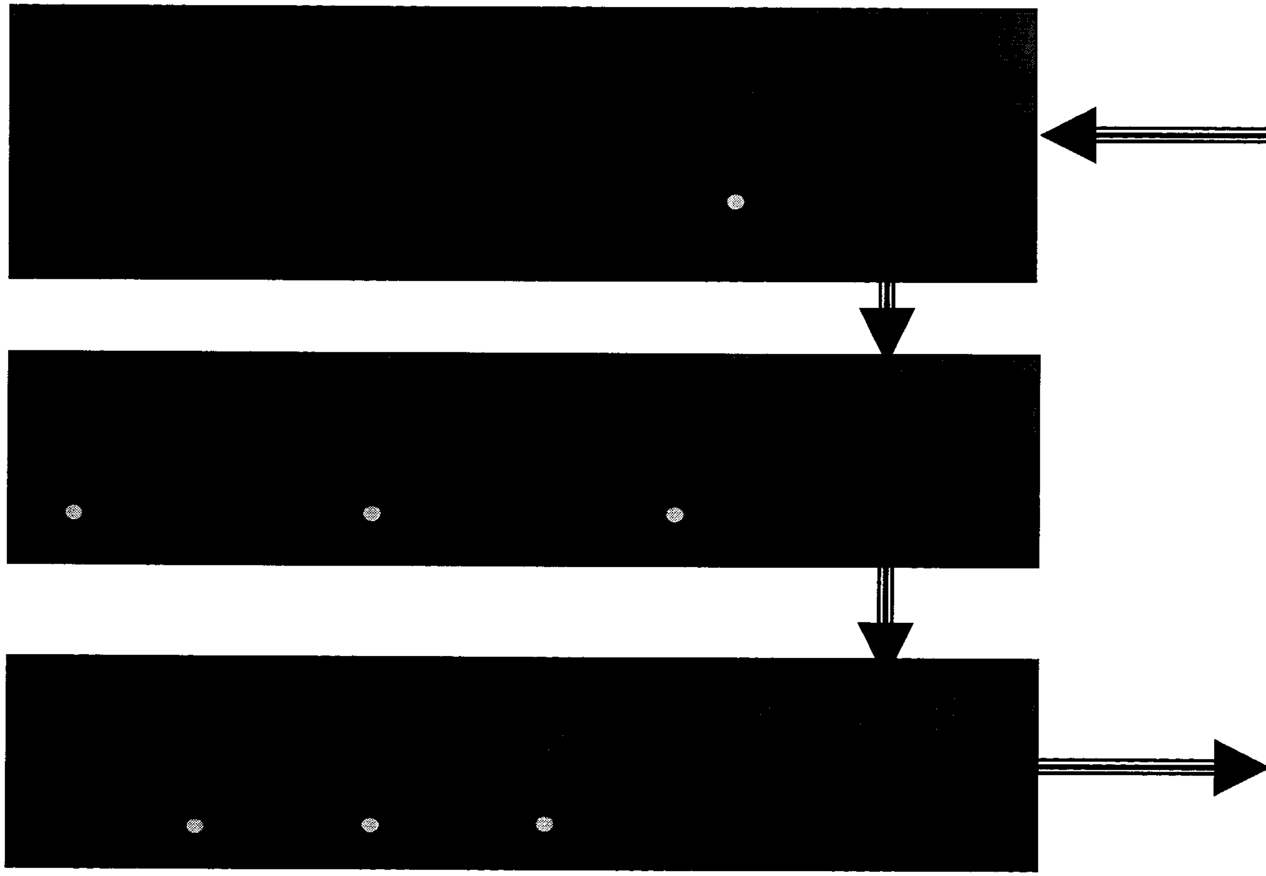
Major portions of this presentation review material developed and published in 1993-1998 at Texas Instruments and Raytheon in Dallas, Texas.

Acknowledgements

- NEMO was developed under a government contract to Texas Instruments and Raytheon from 1993-1997
  - Theory
    - Roger Lake, Chris Bowen, Gerhard Klimeck, Tim Boykin (UAH)
  - Graphical User Interface
    - Dan Blanks, Gerhard Klimeck
  - Programming Approach, Philosophy, and Prototypes
    - Bill Frensley (UTD), Gerhard Klimeck, Chris Bowen
  - Coding Help
    - Manhua Leng (UTD), Chenjing Fernando, Paul Sotirelis, Dejan Jovanovic, Mukund Swaminathan (UTA)
  - Experiments for verification
    - Ted Moise, Alan Seabaugh, Tom Broekaert, Berinder Brar, Yung-Chung Kao

- NEMO 3-D is being developed (1998-...) at JPL by Chris Bowen, Fabiano Oyafuso, Tom Cwik and Gerhard Klimeck.

Bandstructure Basics
Electron Conduction in Solids



Gas

Quantum Mechanics
Optical Transitions
Coulomb Repulsion

Physics

Solid

Transport
conductivity, mobility

Devices

- Bands are channels in which electrons move "freely".
- Layers of **different** atoms are deposited with **monolayer** control.
- We can **engineer** the electron **bands**.

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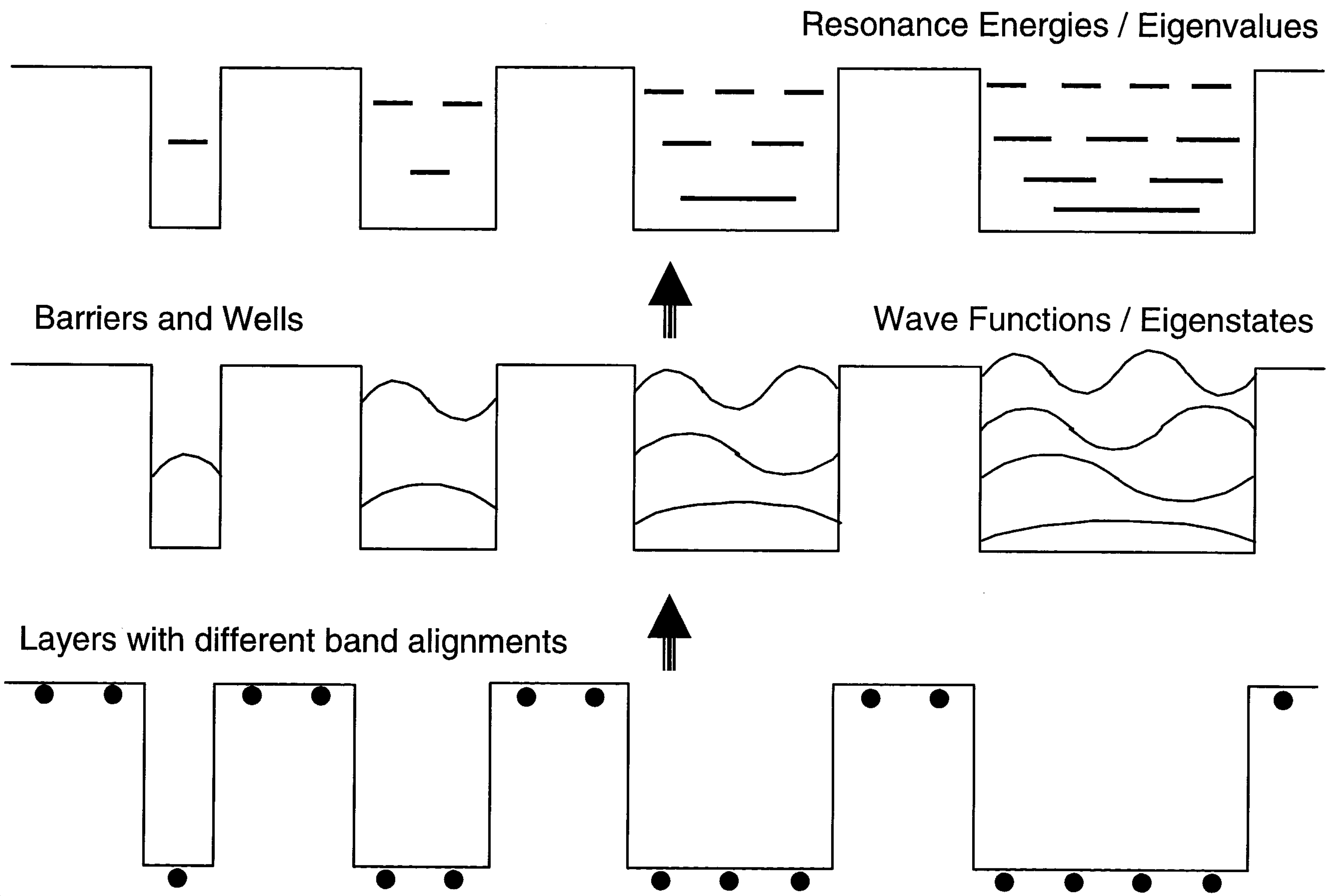
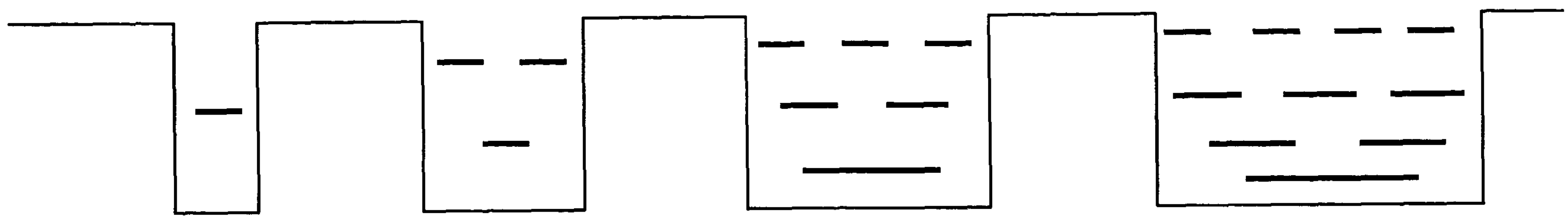
Bandstructure Engineering Basics



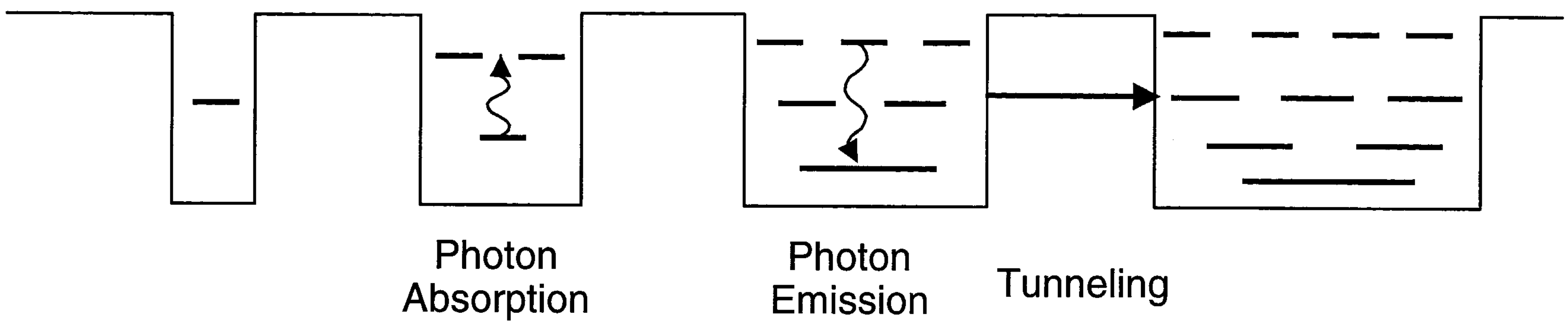
Bandstructure Engineering Basics

Resonance Energies / Eigenvalues



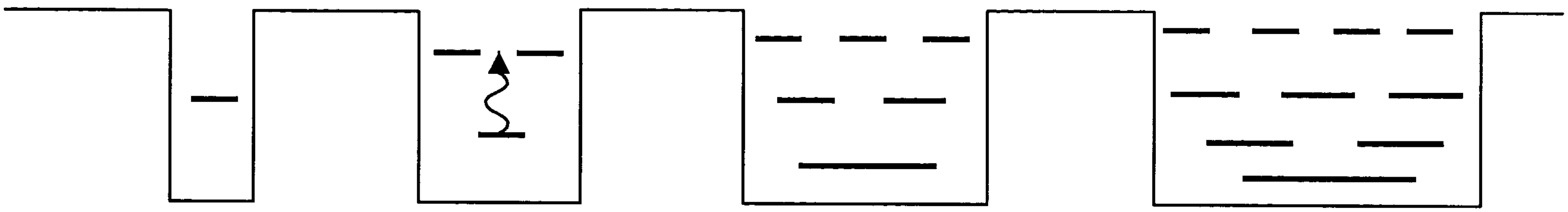
Bandstructure Engineering Applications

Transitions / Transport



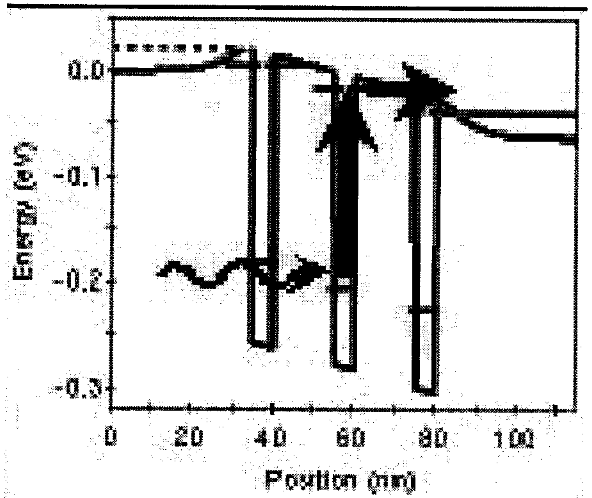
Bandstructure Engineering Applications

Transitions / Transport



Photon Absorption

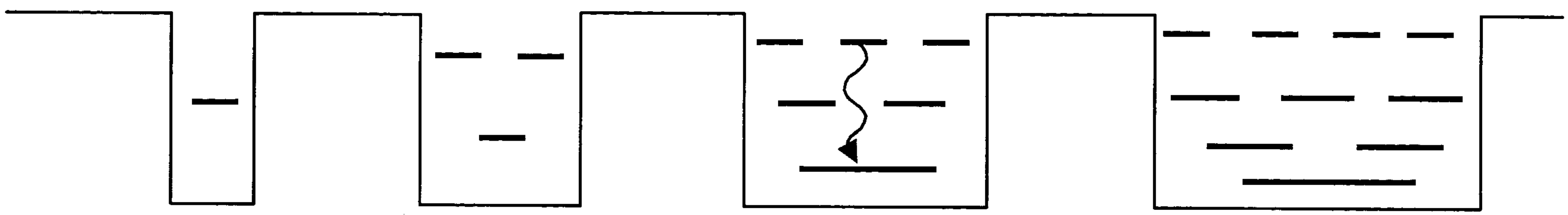
Detectors



Quantum Well Infrared Detector

Bandstructure Engineering Applications

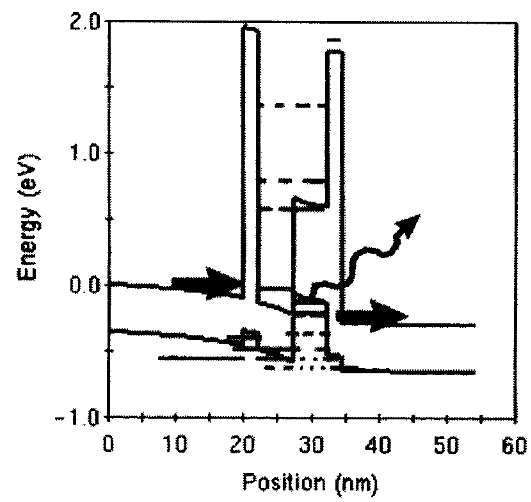
Transitions / Transport



Photon Emission

↓

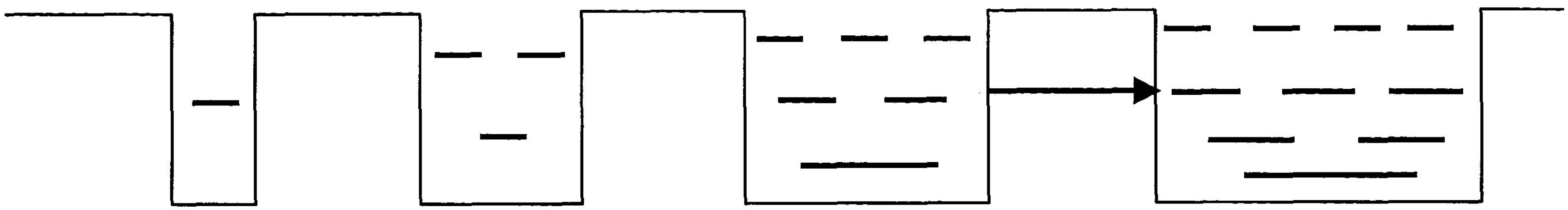
Lasers



Quantum Cascade Laser

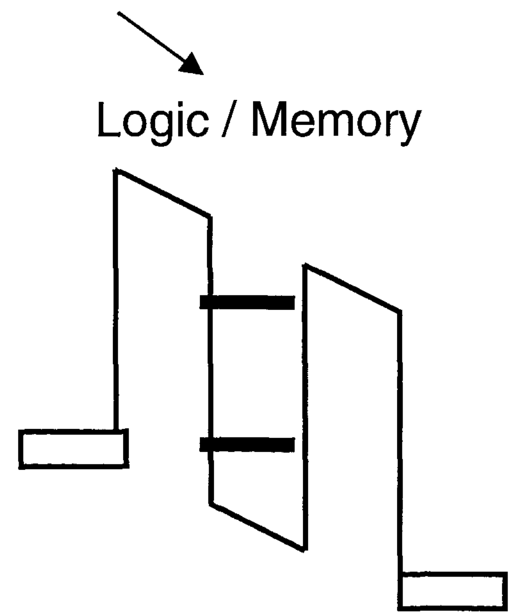
Bandstructure Engineering Applications

Transitions / Transport



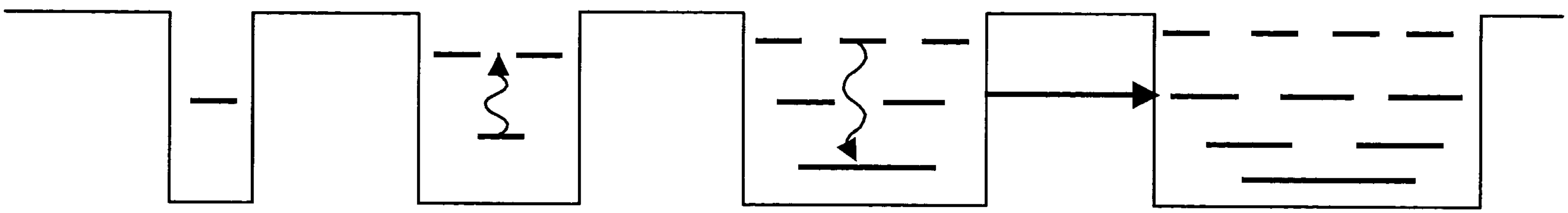
Tunneling

Logic / Memory



Resonant
Tunneling
Diode

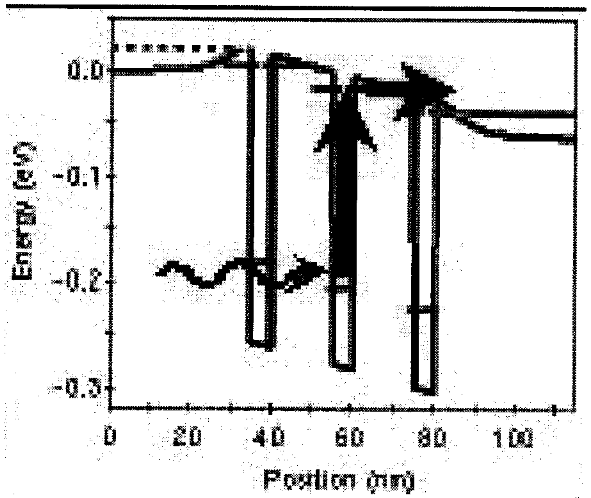
Transitions / Transport Controlled by Design



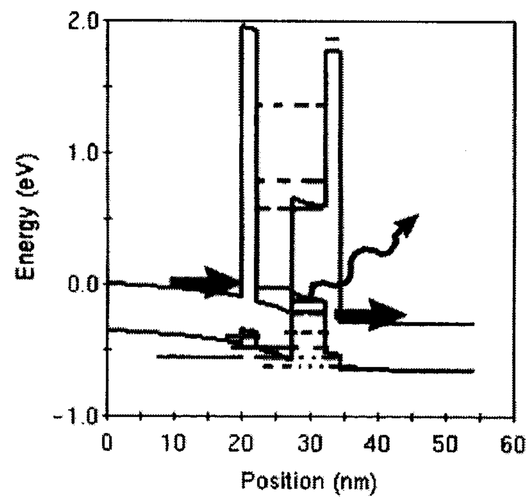
Photon Absorption → Detectors

Photon Emission → Lasers

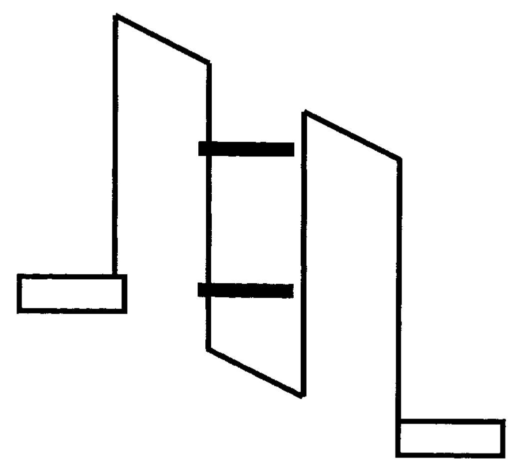
Tunneling → Logic / Memory



Quantum Well Infrared Detector

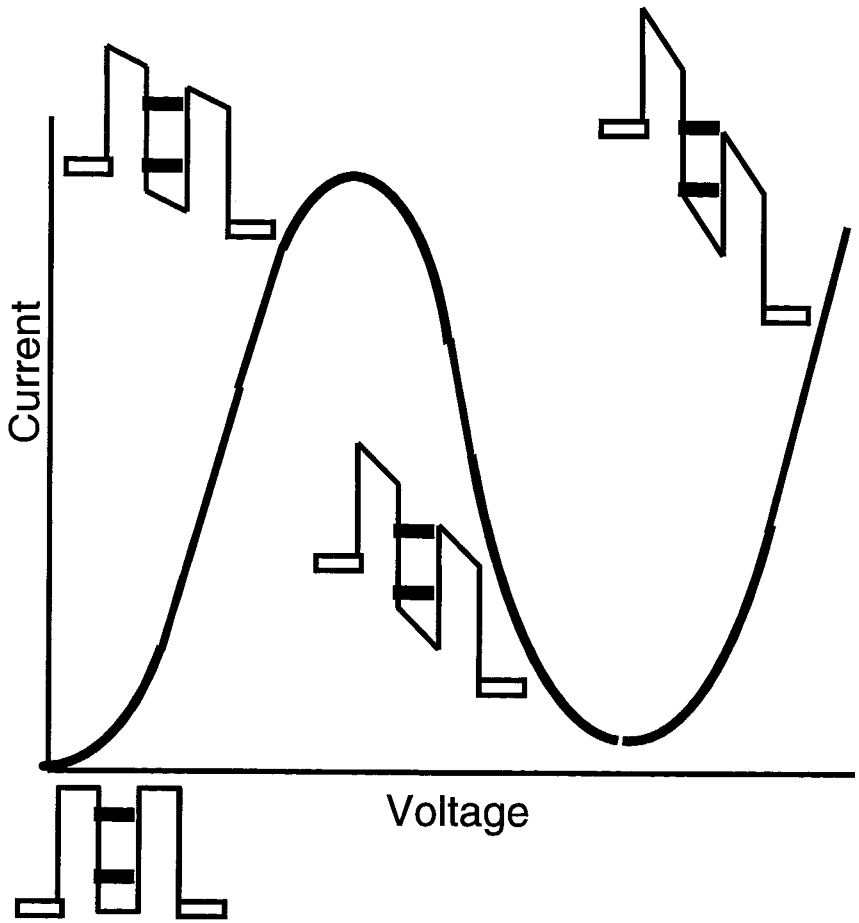


Quantum Cascade Laser

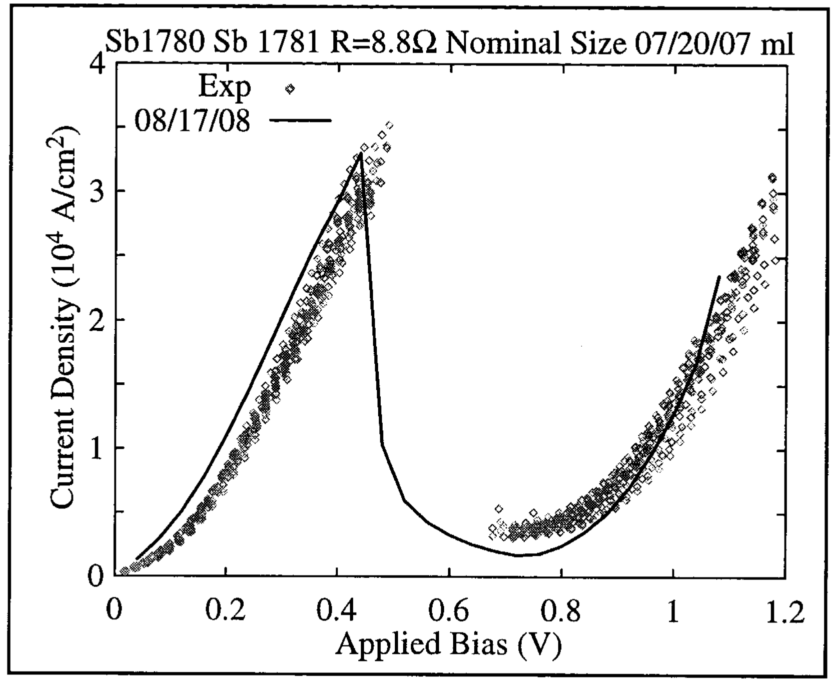


Resonant Tunneling Diode

Resonant Tunneling Diode



Conduction band diagrams for different voltages and the resulting current flow.

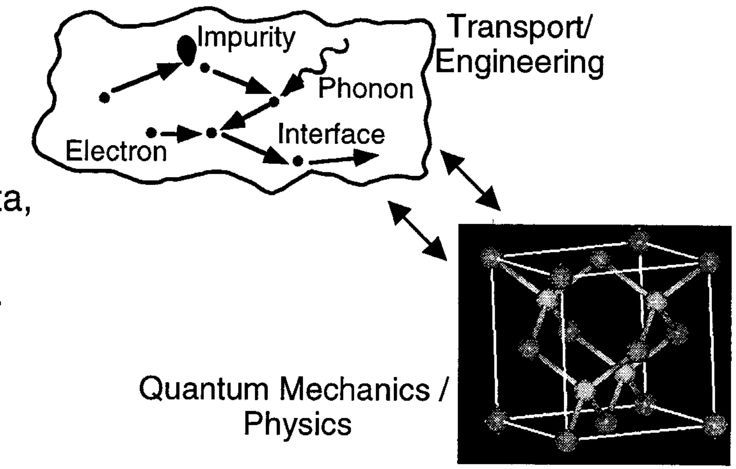


12 different I-V curves: 2 wafers, 3 mesa sizes, 2 bias directions

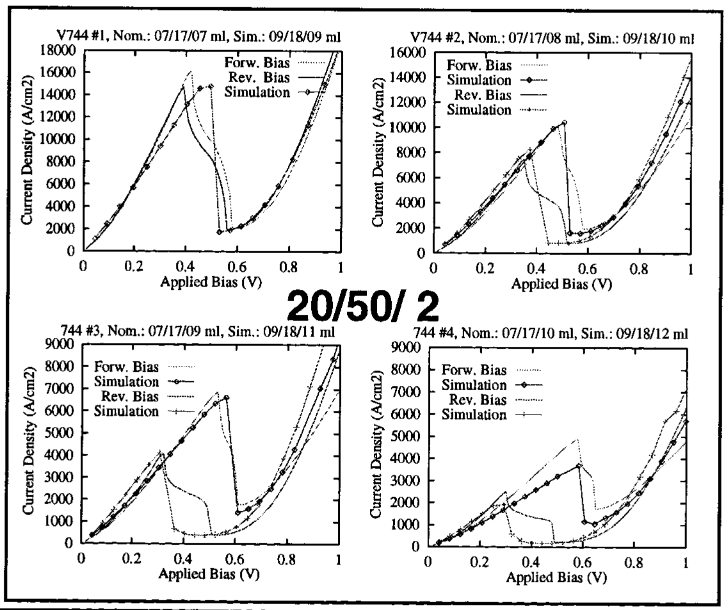
50nm	1e18	InGaAs
7 ml	nid	InGaAs
7 ml	nid	AlAs
20 ml	nid	InGaAs
7 ml	nid	AlAs
7 ml	nid	InGaAs
50 nm	1e18	InGaAs

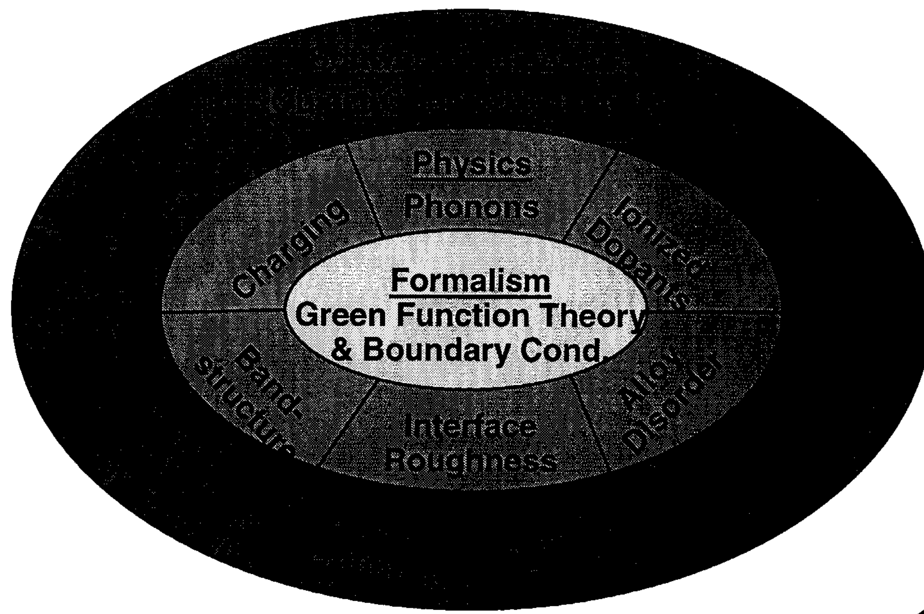
NEMO 1-D: A User-friendly Quantum Device Design Tool

- NEMO was developed under a government contract to Texas Instruments and Raytheon from 1993-97
  - >50,000 person hours of R&D
  - 250,000 lines of code in C, FORTRAN and F90
- Based on Non-Equilibrium Green function formalism (Datta, Lake, Klimeck).
- NEMO in THE state-of-the-art heterostructure design tool.
- Used at Intel, Motorola, HP, Texas Instruments, and >10 Universities.

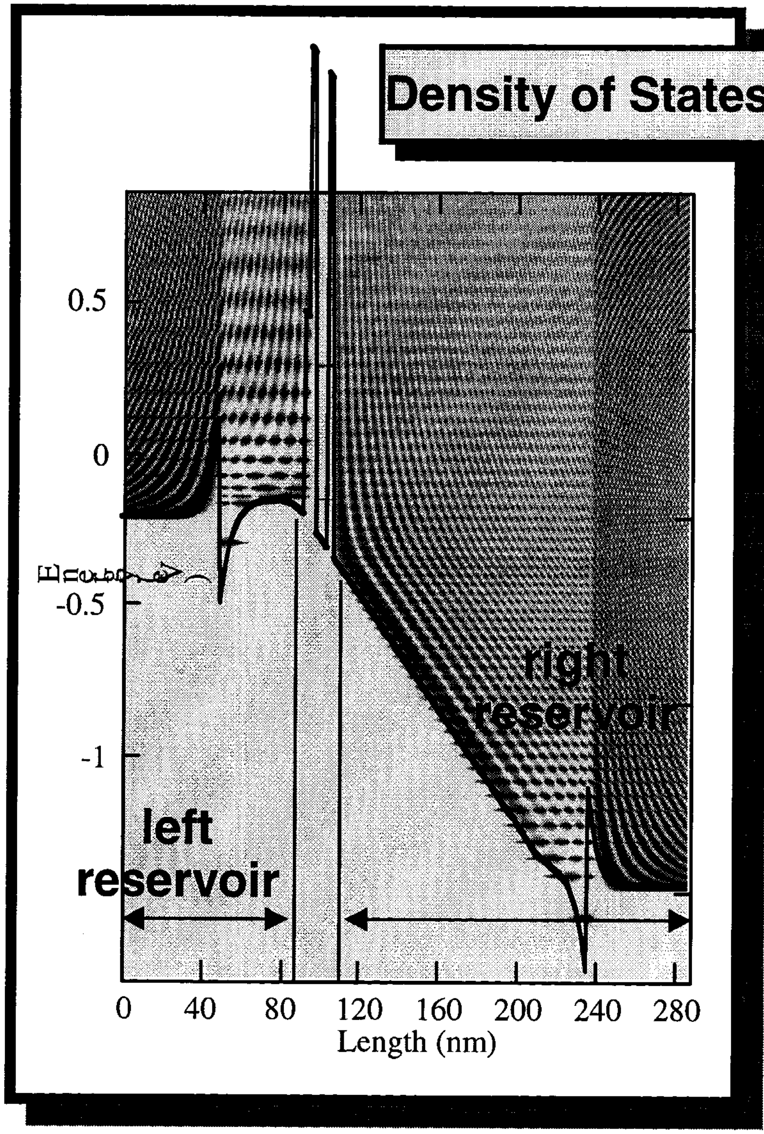


Testmatrix

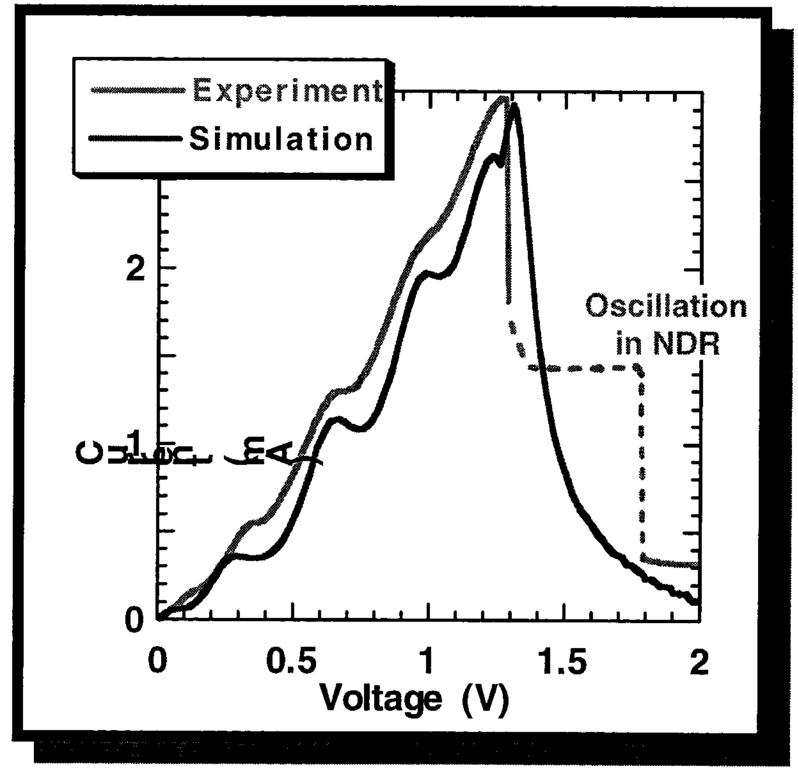




Realistic Devices Have a Large Extent!!!



Quantum Optical Switch



Calculate charge self-consistently in
- **the left and right reservoir**
- **central device region**

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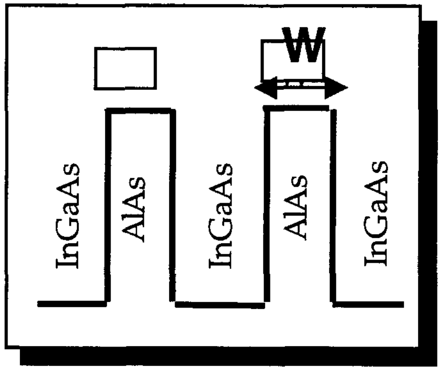
Testmatrix-Based Verification (room temperature)

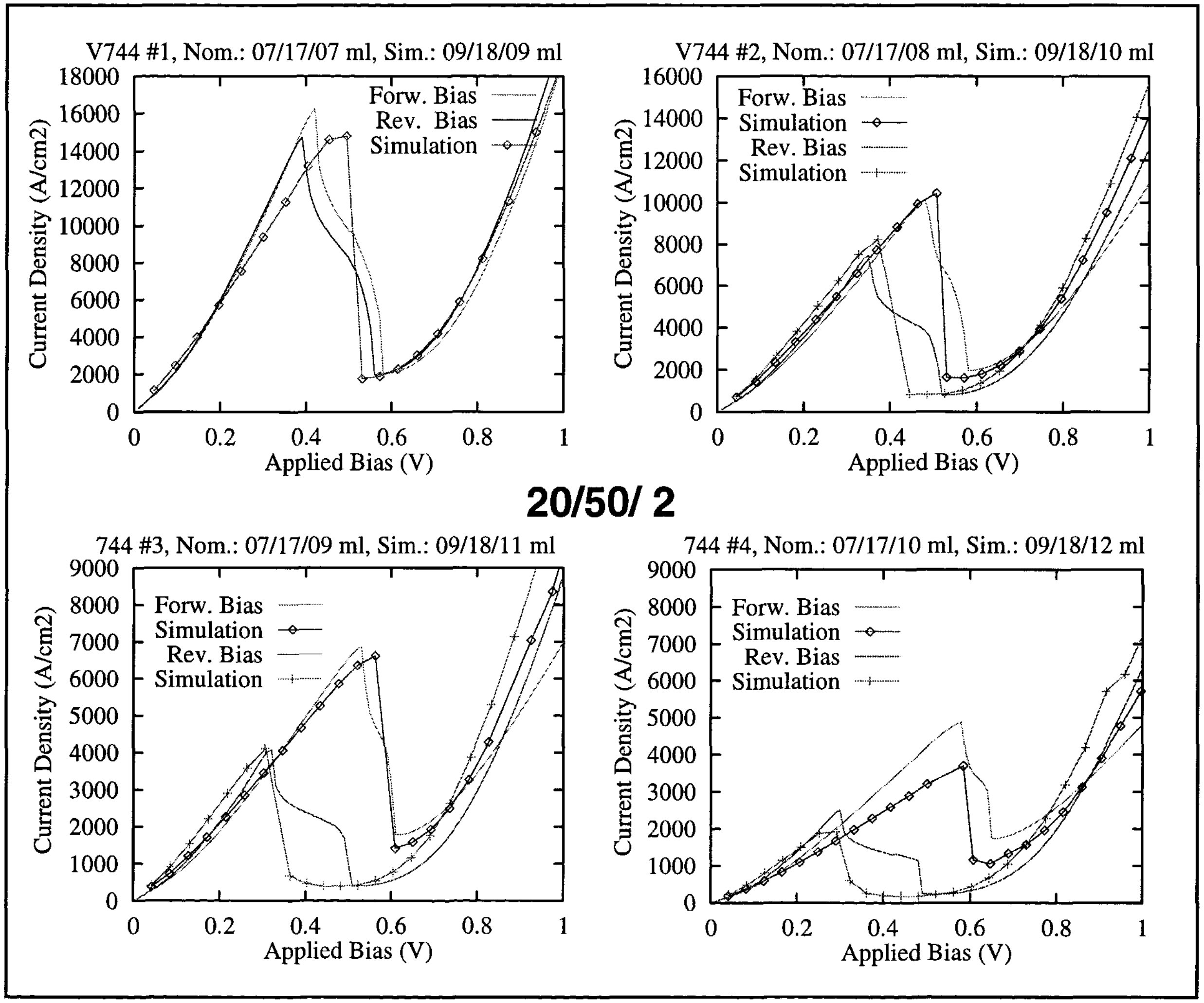
Strained InGaAs/AlAs 4 Stack RTD with Asymmetric Barrier Variation

Vary One Barrier Thickness



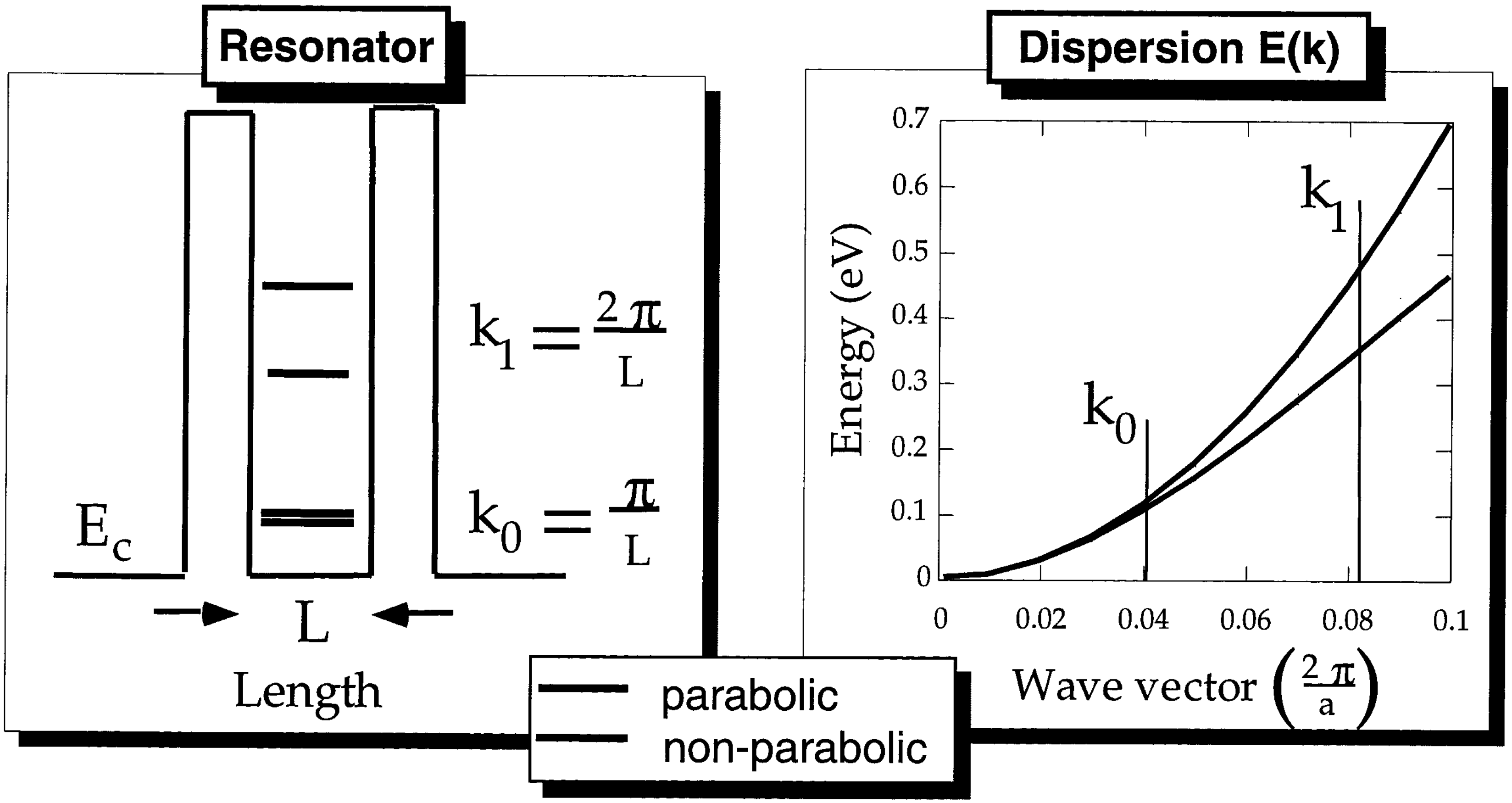
Four increasingly asymmetric devices:

20/50/20 Angstrom
20/50/23 Angstrom
20/50/25 Angstrom
20/50/27 Angstrom



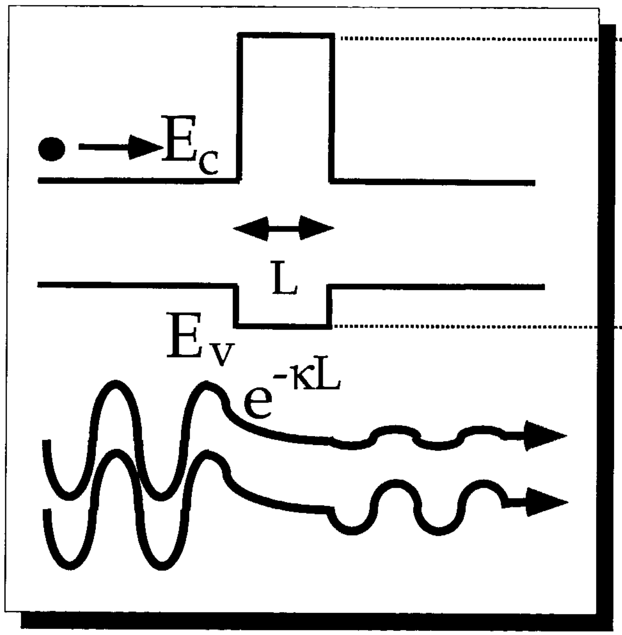
Presented at IEEE DRC 1997, work performed at Texas Instrument, Dallas

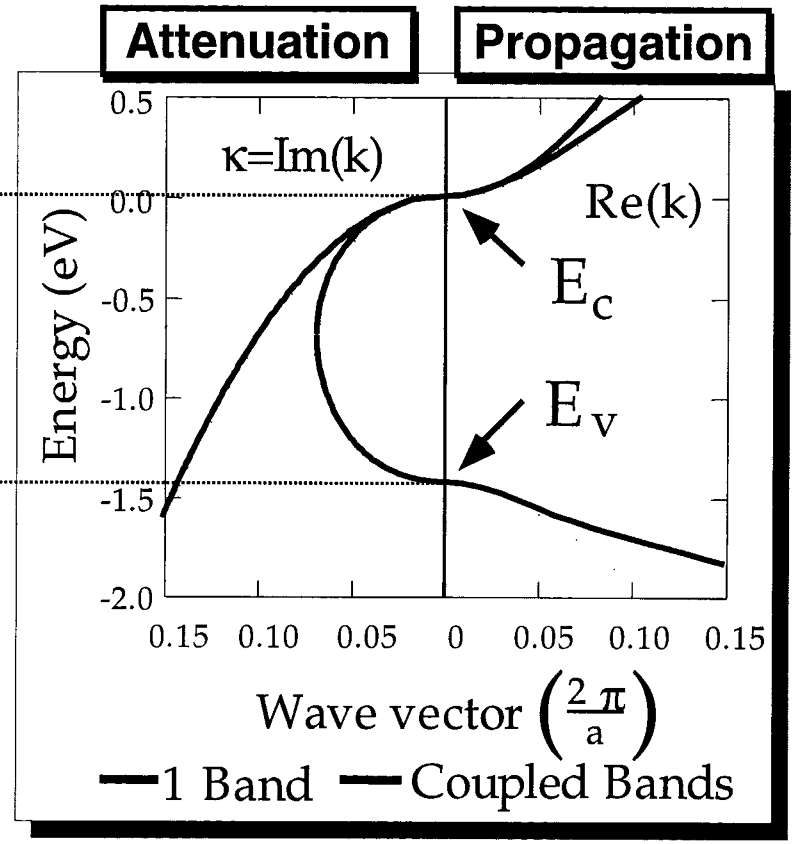
Resonance State Lowering due to Band Non-Parabolicity



Second diode turn-on at lower voltages.

Wave Attenuation in Barriers





- Attenuation is smaller with coupled bands
- Tunneling probability increases
- Current increases

Transport via Transmission Coefficients

$$I \propto \int dk_x \int dk_y \int dE\, T\left(E, k_x, k_y\right)\left(f_L(E) - f_R(E)\right)$$

↓ **Cylindrical Coordinates**

$$I \propto \int d\varphi \int k\,dk \int dE\, T(E, k, \varphi)\left(f_L(E) - f_R(E)\right)$$

↓ **Throw out angular dependence**

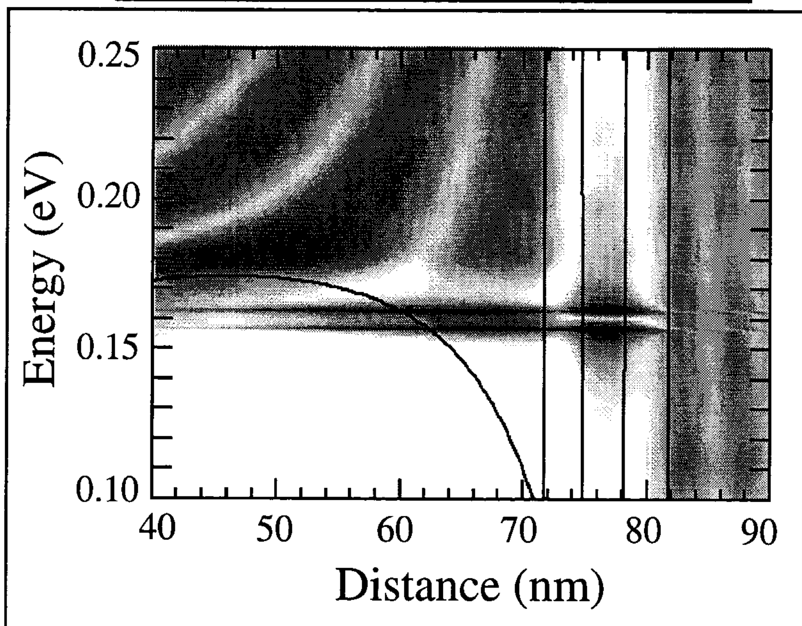
$$I \propto 2\pi \int k\,dk \int dE\, T(E, k)\left(f_L(E) - f_R(E)\right)$$

↓ **Parabolic transverse subbands**

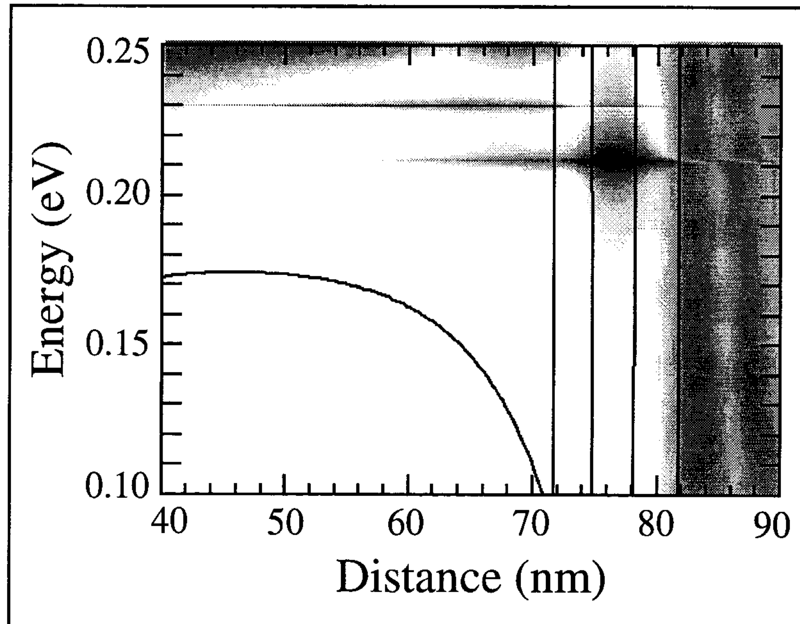
$$I \propto \rho_{2D} \int T(E)\left(f_L(E) - f_R(E)\right)$$

Resonance Coupling vs. Transverse Momentum

Density of States (k_x=0.00)

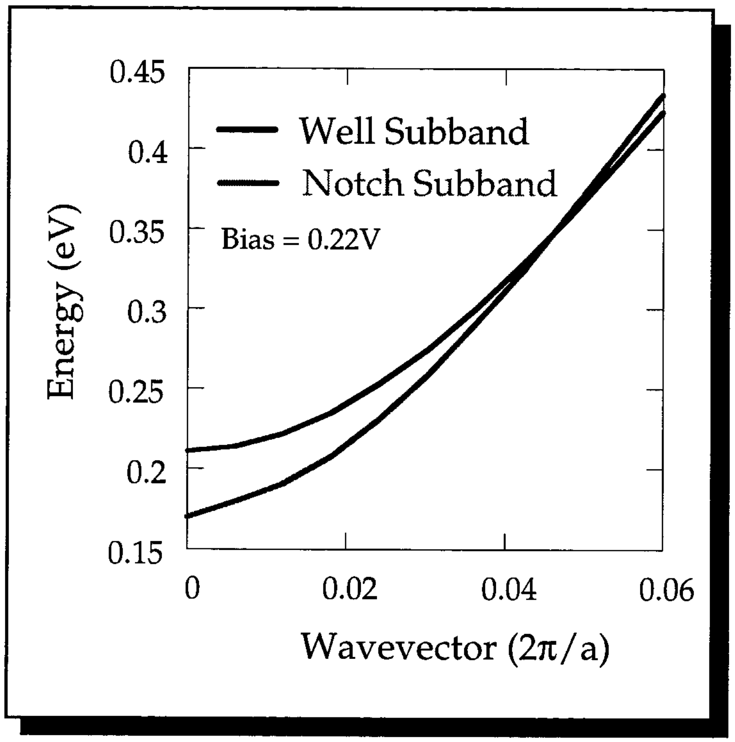


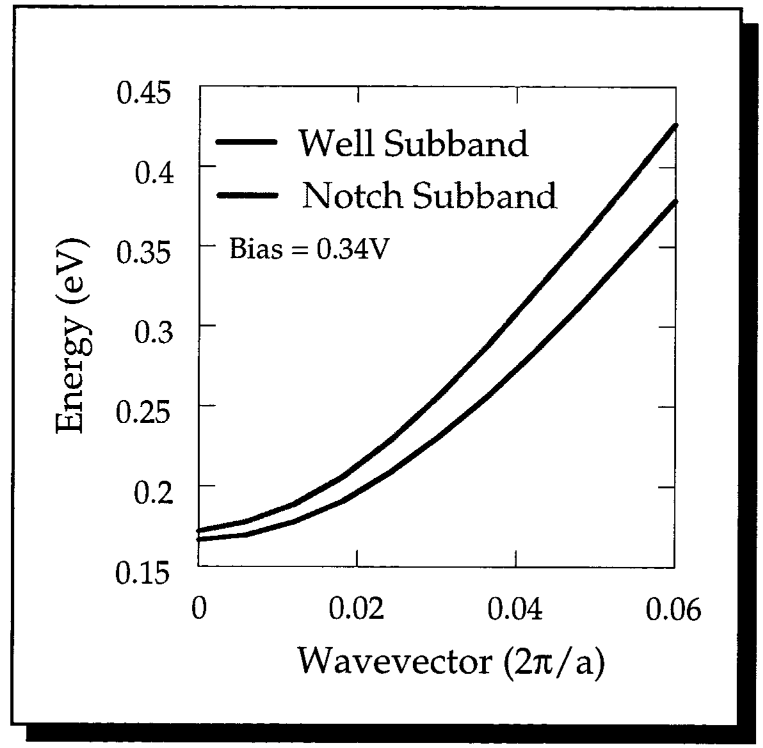
Density of States (k_x=0.03)



Resonance coupling depends on the transverse momentum

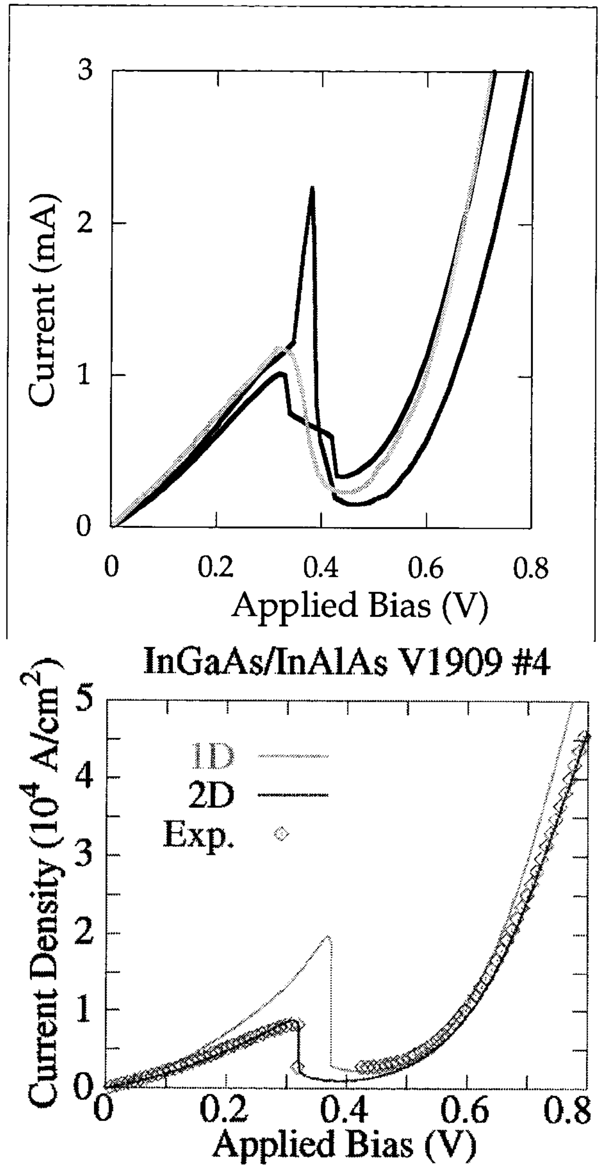
Quantum Well and Notch Subbands





- The dispersions are non-parabolic
- There is no "perfect" overlap of the subbands

Full Band Simulation of Electron Transport

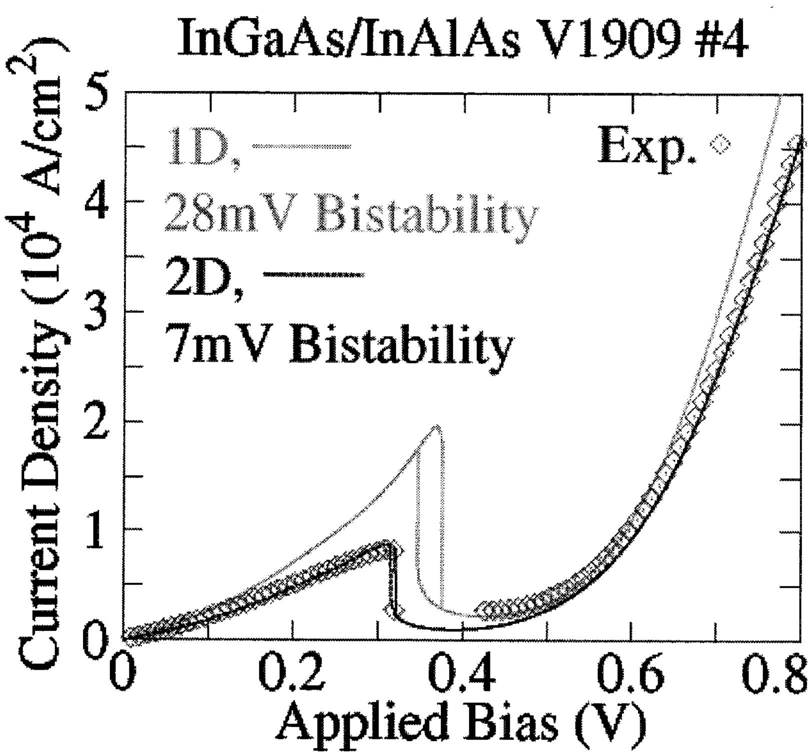


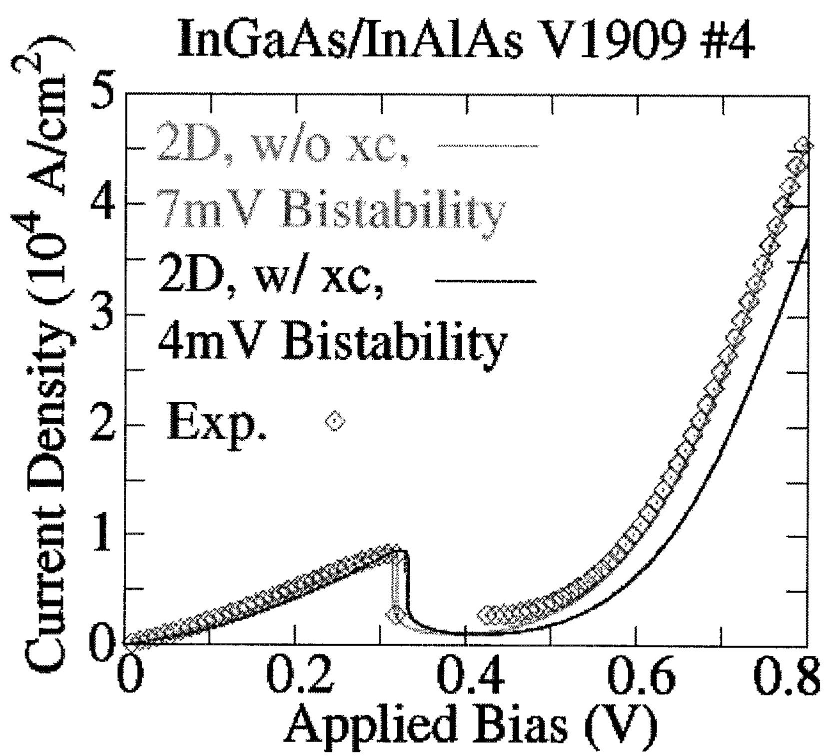
- 1D integration assuming parabolic subbands can lead to unphysical current overshoots.
- 2 Examples on InGaAs/InAlAs simulations:
  - Sp3s* simulation with partial charge self-consistency
    -> sharp spike at turn-off
  - Parameterized single band simulation which incorporates the band-non-parabolicity
    -> overall current overshoot.

- -> 2D integration fixes these unphysical results.

More Physics -> Better results

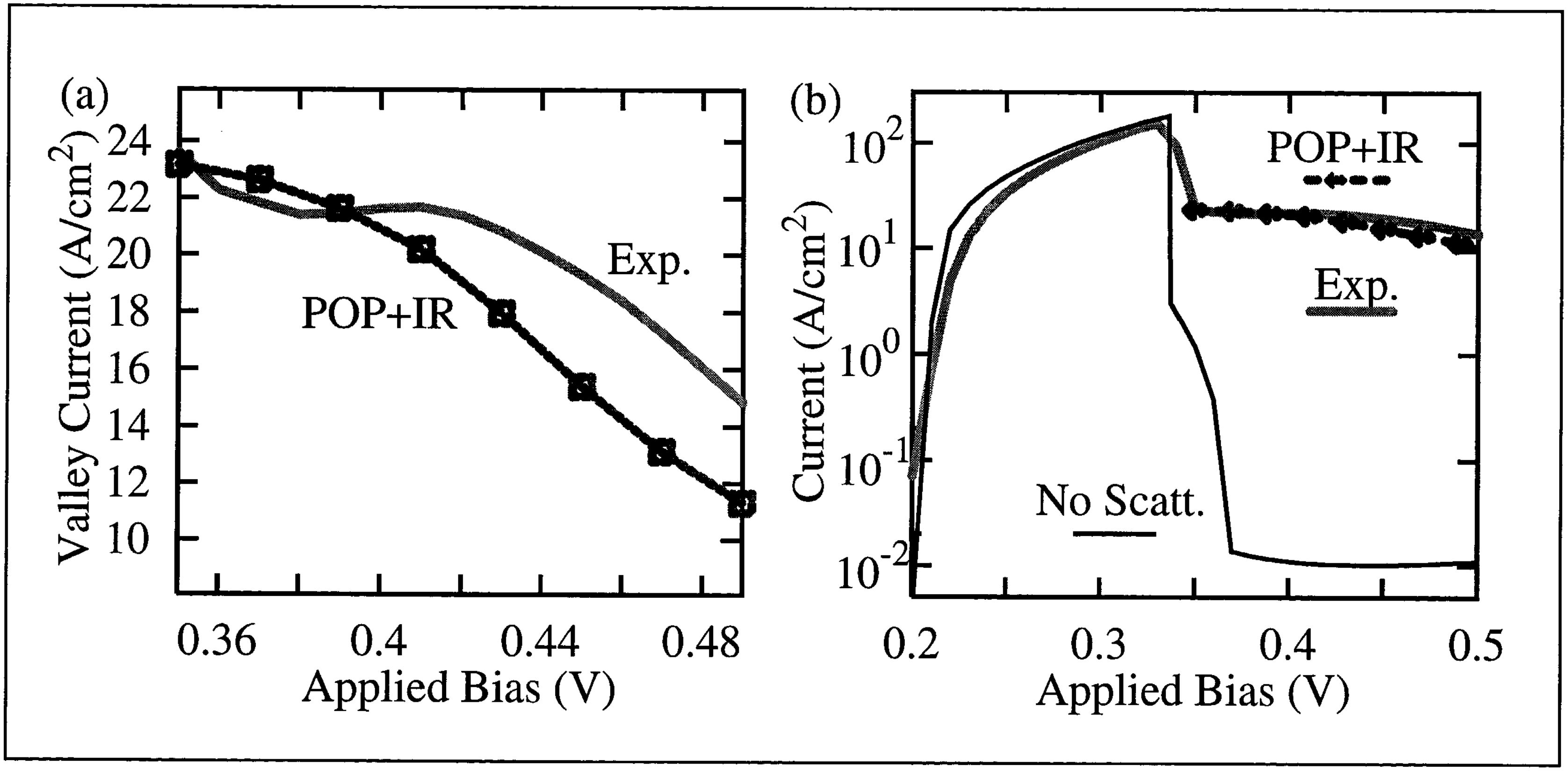
Full band integration + Exchange&Correlation





- Calculate the exchange and correlation potential in the local density approximation.
- Exchange and correlation energy does not eliminate (in general) the bistability, it does reduce it however.
- Inclusion of scattering in the simulation reduces the bistability region as well.

Tow Temperature: Polar Optical Phonon and Interface Roughness Scattering



scattering raises valley current by several orders of magnitude

Optical/E&M Analogies to Quantum Mech.

$$\nabla^2 \vec{E} = -\omega^2 \mu \varepsilon \vec{E}$$

$$k^2 = \omega^2 \mu \varepsilon$$

$$\nabla^2 \Psi = -\frac{2m}{\hbar}(E-U)\Psi$$

$$k^2 = \frac{2m}{\hbar}(E-U)$$

Physics are similar:

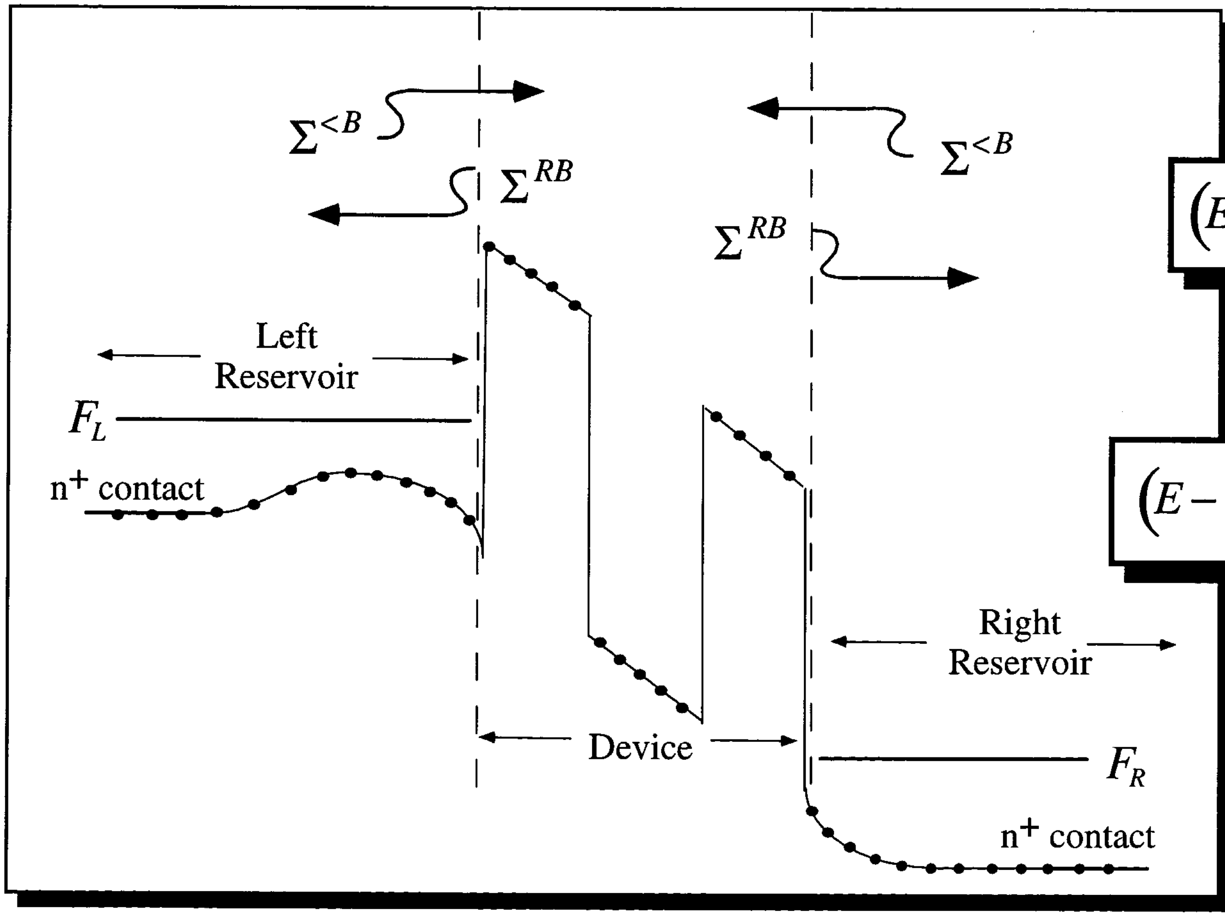
- Propagation as a wave phenomenon:
  - Antennas
  - Waveguides
- Propagation as a scattering problem:
  - Diffraction gratings
  - Radar cross-sections
- Green functions as propagators
- Finite difference, finite elements

But:

- Scattering is coherent & elastic rather than incoherent & inelastic
- Photons do not interact with themselves:
  - Calculate the propagation
  - Do not calculate the occupation
  - Exception is a laser!
- Electron and Laser Simulation need: Dynamics & Kinetics - States & Bean-counting

Generalized Boundary Conditions: Boundaries as a Scatterong Problem

- Left and right regions are treated as reservoirs.
- Quantum structure of reservoirs is included exactly.



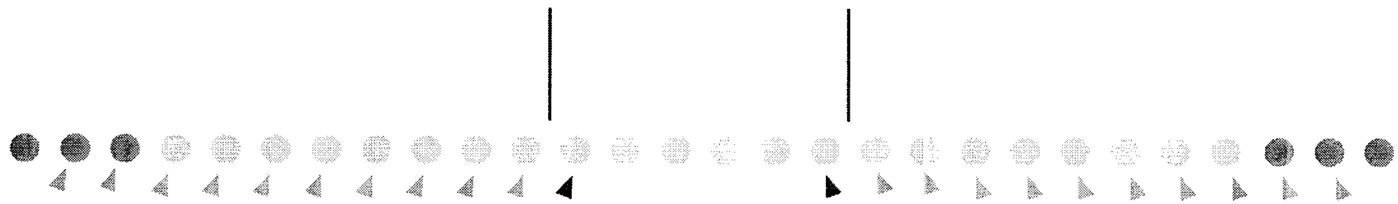
Dynamics

$$\left(E - H_0 - \Sigma^{RB}\right)G^R = 1$$

$$\left(E - H_0 - \Sigma^{RB}\right)G^< = \Sigma^{<B}G^A$$

Kinetics

Dyson Equation Treatment of the Leads



$$\Sigma^{RB}_{0,0} = g^{R}_{-1,-1}\left|t_{-1,0}\right|^2$$

$$\Sigma^{RB}_{N-1,N-1} = g^{R}_{N,N}\left|t_{N,N-1}\right|^2$$

$$\Sigma^{<B}_{0,0} = -2\ \mathrm{IM}\ \left\{\Sigma^{RB}_{0,0}\right\} f_L$$

$$\Sigma^{<B}_{N-1,N-1} = -2\ \mathrm{IM}\ \left\{\Sigma^{RB}_{N-1,N-1}\right\} f_R$$

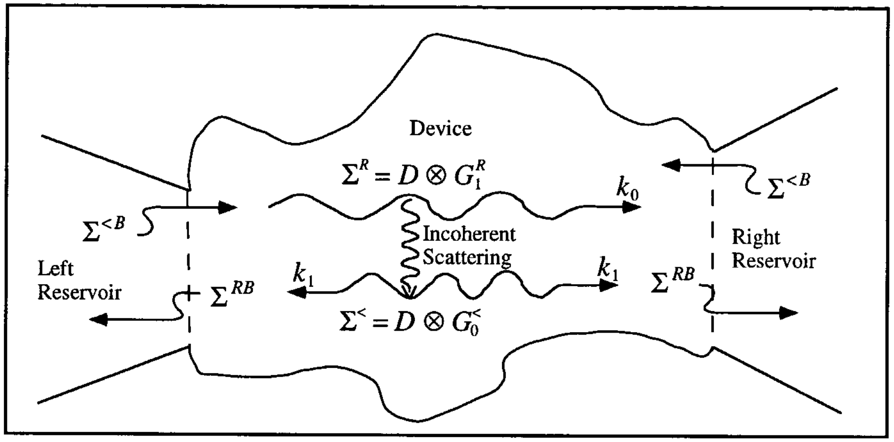
$$\left[G^R\right]^{-1} = \begin{bmatrix} E-\varepsilon_0-\Sigma^R_{0,0} & t_{0,1} & & \\ t_{1,0} & E-\varepsilon_1 & \mathrm{O} & \\ & \mathrm{O} & \mathrm{O} & \\ & & & E-\varepsilon_{N-1}-\Sigma^R_{N-1,N-1} \end{bmatrix}^{-1}$$

$$\left(E-H_0-\Sigma^{RB}\right)G^R = 1$$

Dynamics → **Kinetics**

$$\left(E-H_0-\Sigma^{RB}\right)G^< = \Sigma^{<B}G^A$$

Treatment of a single Incoherent Scattering Event



- **Scattering:**
  - **couples different propagation channels (k and E).**
  - **modifies the quantum mechanical spectrum of states (damped oscillator has a different eigen frequency)**
- **Incoherent Scattering:**
  - **Destroys phase memory**

$$(E - H_o^D - \Sigma^{RB})G_1^R = 1$$

↓

$$\Sigma_0^R = D \otimes G_1^R$$

↓

$$(E - H_o^D - \Sigma^{RB} - \Sigma_0^R)G_0^R = 1$$

↓

$$G_0^< = G_0^R \Sigma^{<B} G_0^A$$

↓

$$\Sigma_0^< = D \otimes G_0^<$$

↓

$$G_1^< = G_1^R \Sigma_0^< G_1^A$$

Computation ↓

Transport ↑

Multiple Sequential Scattering

Begin with calculations of bare Green function for all transverse k.

$$G_0^R(E) = \left[E - H_o^D\right]^{-1}$$
$$\sigma_0^R(E) = D_{el} \otimes G_0^R(E)$$

$$G_1^R(E) = \left[E - H_o^D - \sigma_0^R(E)\right]^{-1}$$
$$\sigma_1^R(E) = D_{el} \otimes G_1^R(E)$$

⋮

$$G_{N-1}^R(E) = \left[E - H_o^D - \sigma_{N-2}^R(E)\right]^{-1}$$
$$\sigma_{N-1}^R(E) = D_{el} \otimes G_{N-1}^R(E)$$

$$G_N^R(E) = \left[E - H_o^D - \sigma_{N-1}^R(E)\right]^{-1}$$

$$G_N^<(E) = G_N^R(E)\Sigma^{<B}(E)G_N^A(E)$$
$$\sigma_N^<(E) = D_{el} \otimes G_N^<(E)$$

$$G_{N-1}^<(E) = G_{N-1}^R(E)\sigma_N^<(E)G_{N-1}^A(E)$$
$$\sigma_{N-1}^<(E) = D_{el} \otimes G_{N-1}^<(E)$$

⋮

$$G_1^<(E) = G_1^R(E)\sigma_2^<(E)G_1^A(E)$$
$$\sigma_1^<(E) = D_{el} \otimes G_1^<(E)$$

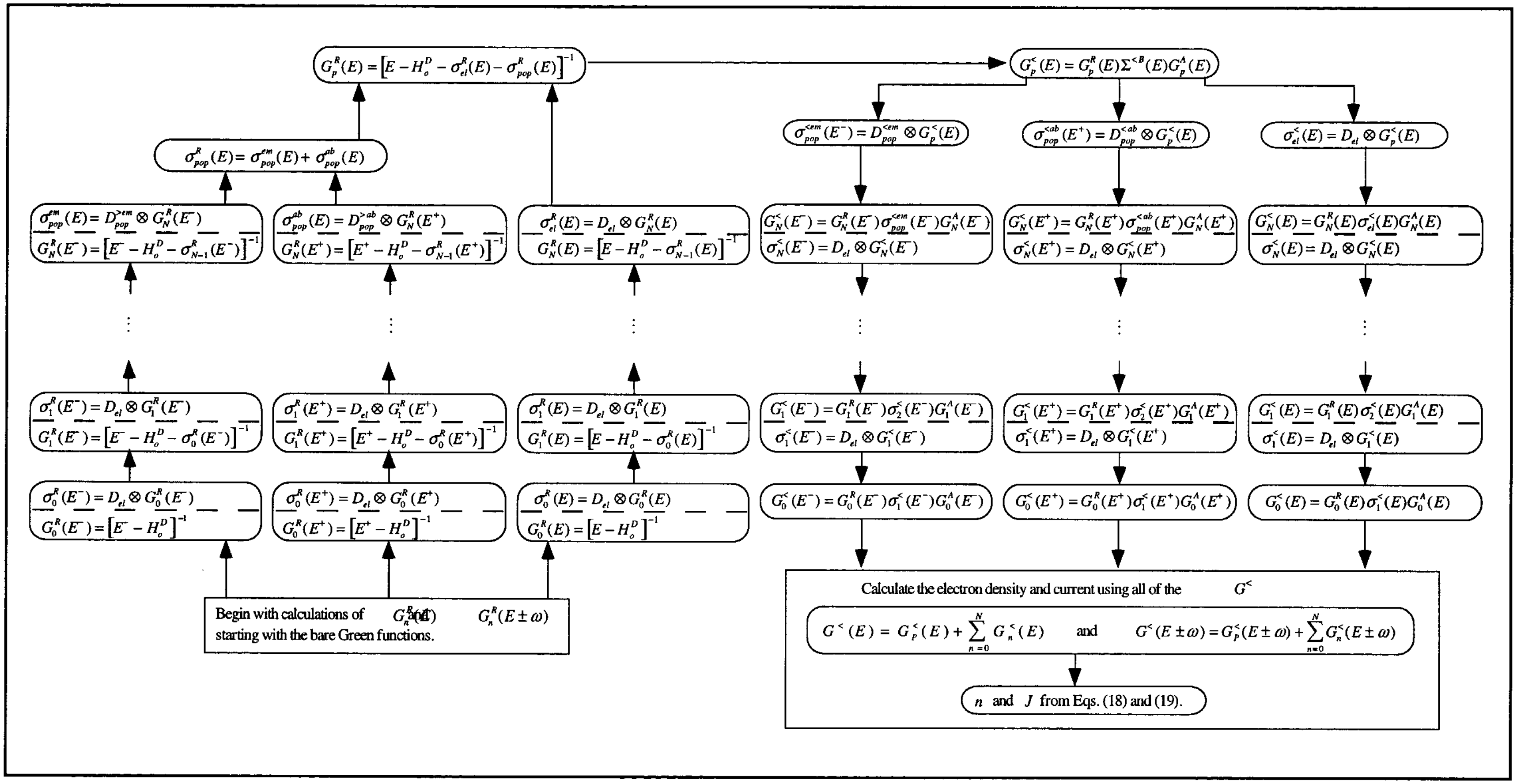
$$G_0^<(E) = G_0^R(E)\sigma_1^<(E)G_0^A(E)$$

Calculate the electron density and current using all of the $G^<$

$$G^<(E) = \sum_{n=0}^{N} G_n^<(E)$$

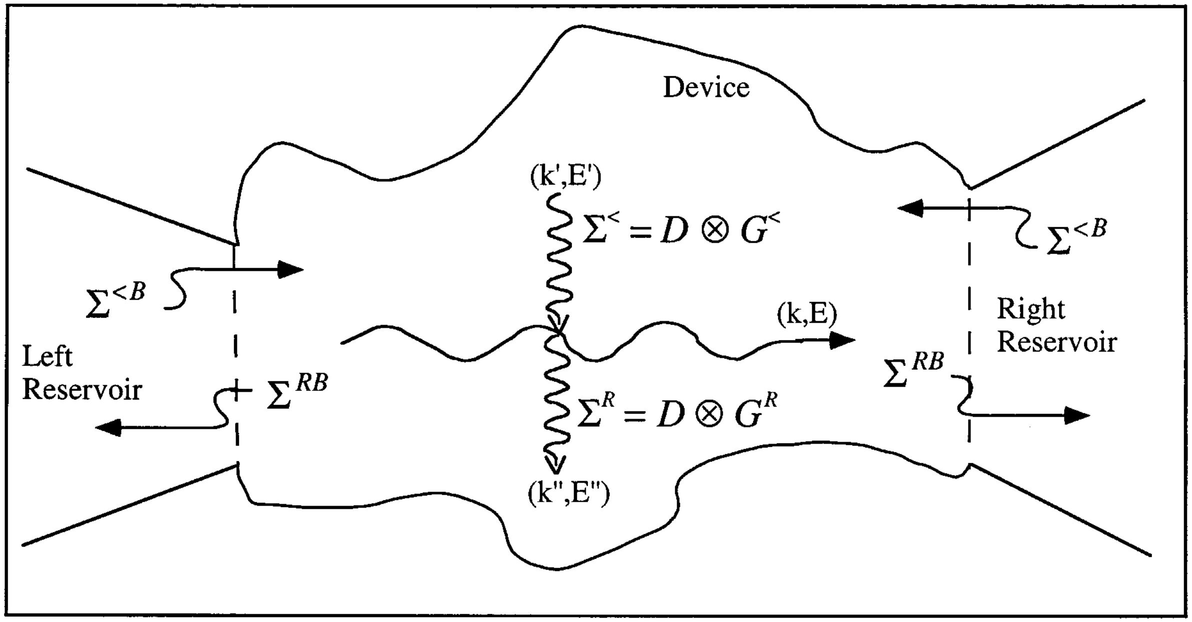
$n_L(E)$ and $J_L(E)$ from Eqs. (18) and (19).

Multiple Sequential Scattering with POP



- Elastic scattering couples all momenta (k)
- Inelastic scattering couples different total energies (E,E+hv,E-hv)
- Polar optical phonons are treated as a single scattering event in NEMO

Scattering: Self-Consistent Born Treatment



Dynamics

$$\left(E - H_0 - \Sigma^{R}_{SCATT} - \Sigma^{R}_{BOUND}\right)G^{R} = 1$$

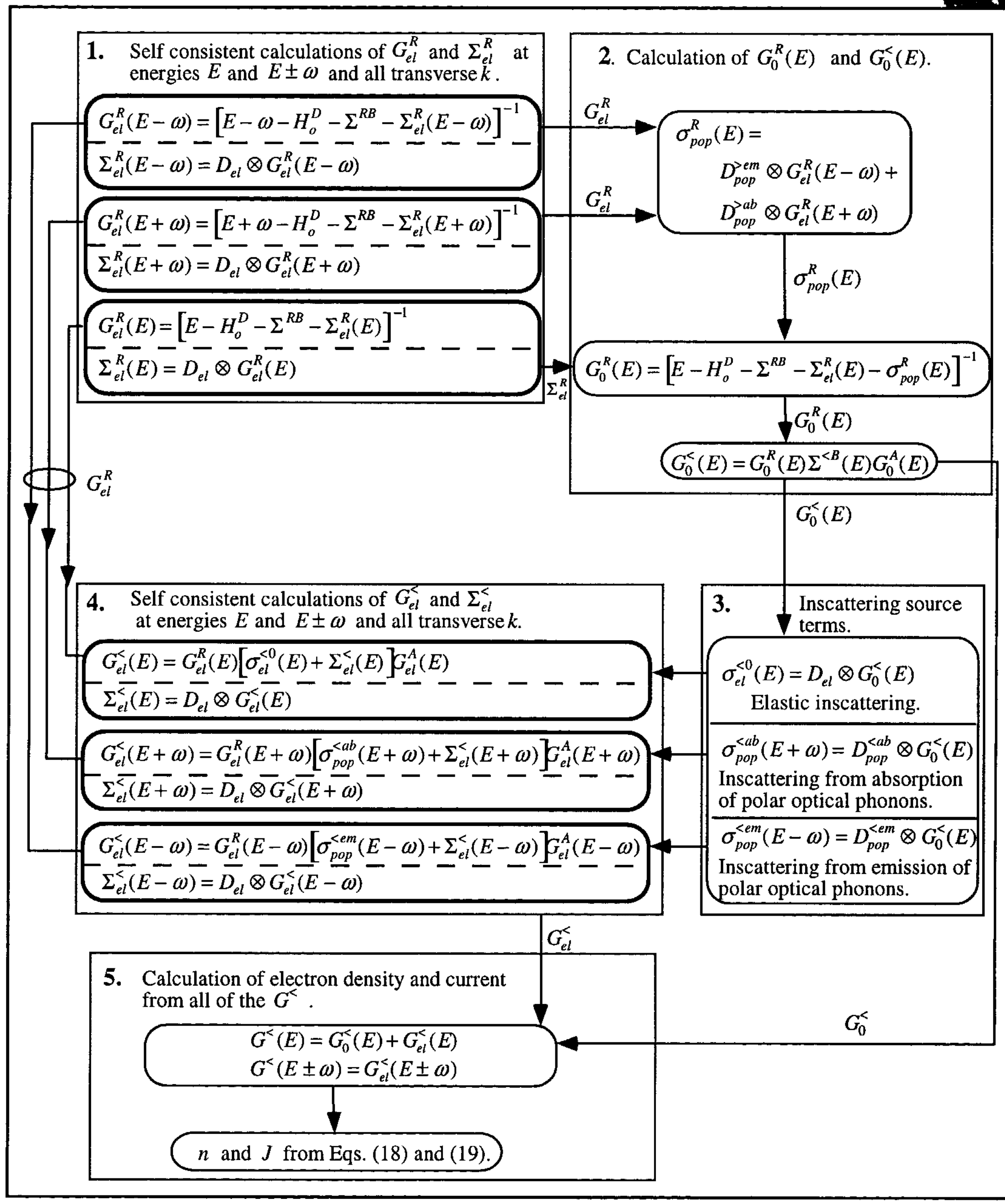
Kinetics

$$\left(E - H_0 - \Sigma^{R}_{SCATT} - \Sigma^{R}_{BOUND}\right)G^{<} = \left(\Sigma^{<}_{SCATT} - \Sigma^{<}_{BOUND}\right)G^{A}$$

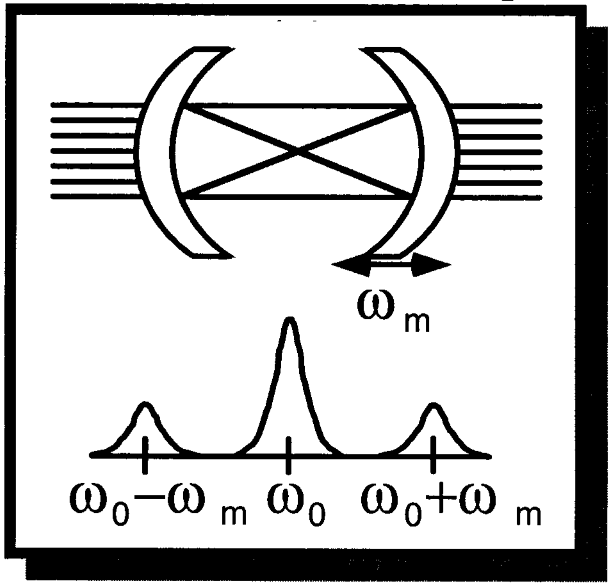
Infinite number of uncorrelated single scattering events.

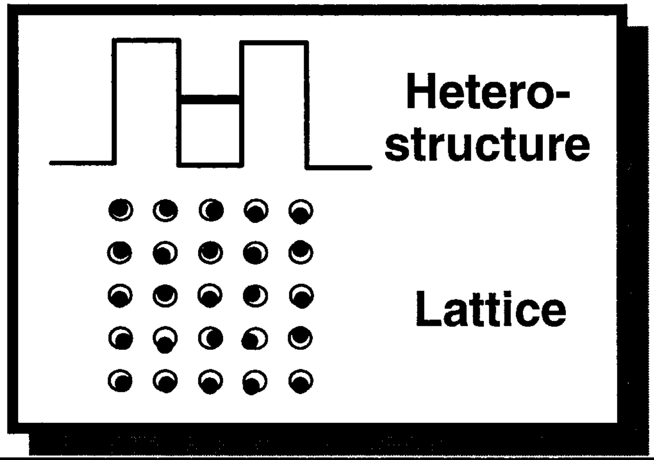
Self-Consistent Born Scattering with POP

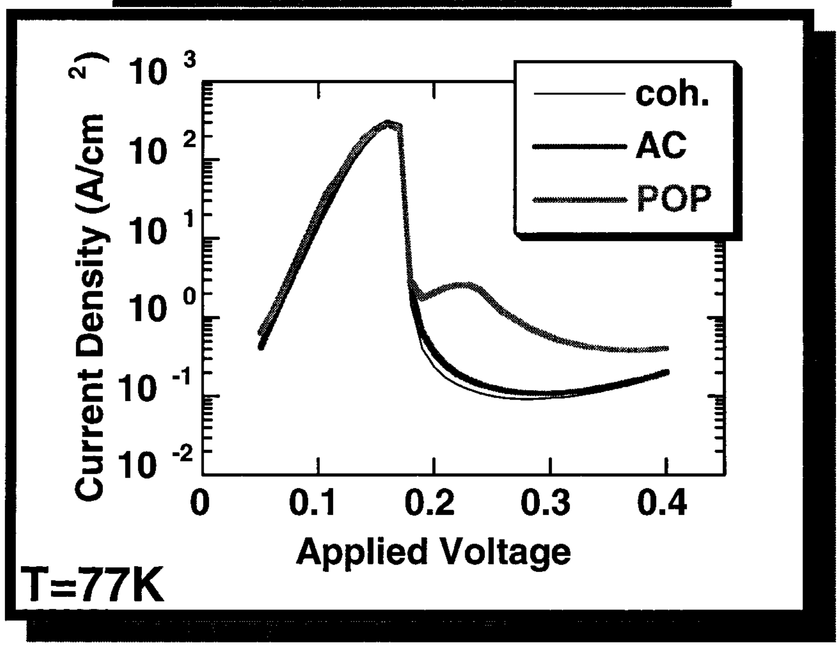
- Elastic scattering couples all momenta (k)
- Inelastic scattering couples different total energies (E,E+hv,E-hv)
- Polar optical phonons are treated as a single scattering event in NEMO



Electron-Phonon Interactions Coupled Resonators







Self-consistent Born (infinite sequential scattering) treatment of acoustic phonon-scattering

Single sequential scattering treatment of polar optical phonon scattering