A Phenomenological Method to Reduce NEGF Simulation from *3D* to *1D* for Lateral Translation Invariant Systems

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Alejo Carpentier: “El Retorno a la Semilla”

StarTrek: “To boldly go where no one has gone before”

Outline (From simple to complex)

- Motivation
- The Method: Ballistic Model

  Simple Models, Boltzmann formula
- Elastic Scattering Model
- Inelastic Scattering, future thoughts
- Recombination Model
- Conclusions

Slide Rule Era

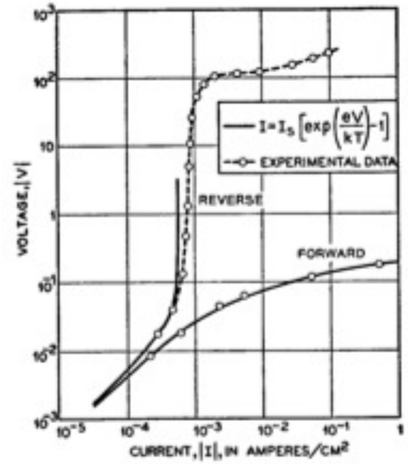


Fig. 4-6—Theoretical Rectification Curve and Experimental Data for a p-n Junction.

Semiconductors (Shockley)

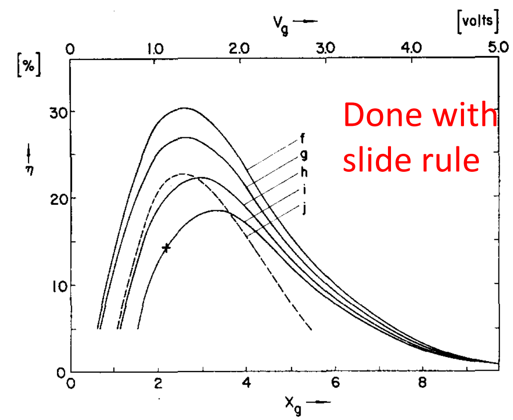


Fig. 6. Efficiency η for a solar cell at temperature $T_c=300°K$ exposed to a blackbody sun at temperature $T_s=6000°K$. Curve (f) is the detailed balance limit of efficiency, assuming the cell is a blackbody (i.e., $t_s=t_c=1$). Curve (j) is the semiempirical limit, or limit conversion efficiency of Prince (see footnote 3). + represents the "best experimental efficiency obtained to date" for Si (see footnote 6). Curves (g), (h), and (i) are modified to correspond to 90% absorption of radiation (i.e., $t_s=t_c=0.9$) and 100-mw incident solar energy. The values for the f quantities discussed in Sec. 6 are: (f) $f=1.09\times10^{-5}$ ($f_\omega=2.18\times10^{-5}$, $f_c=1$) $t_s=t_c=1$; (g) $f=0.68\times10^{-5}$ ($f_\omega=1.36\times10^{-5}$, $f_c=1$) $t_s=t_c=0.9$; (h) $f=0.68\times10^{-8}$ ($f_\omega=1.36\times10^{-5}$, $f_c=10^{-3}$) $t_s=t_c=0.9$; (i) $f=0.68\times10^{-11}$ ($f_\omega=1.36\times10^{-5}$, $f_c=10^{-6}$) $t_s=t_c=0.9$.

Detailed balance (Shockley&Queisser)

Computer era, All atoms count or not ?

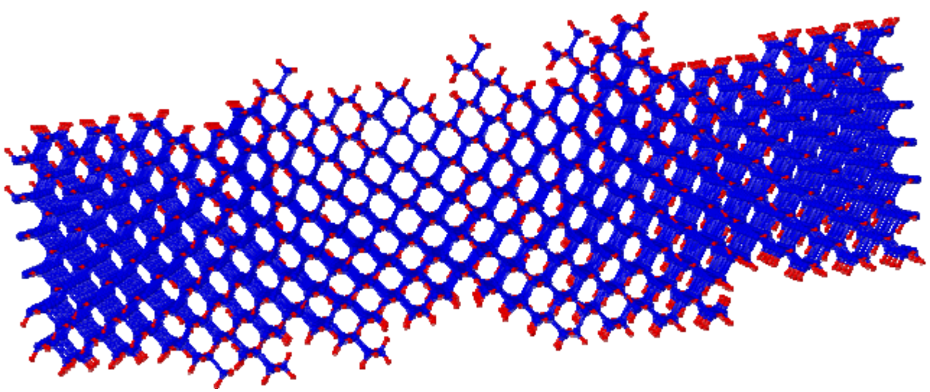


Figure 3. Silicon Nanowire with rough interface passivated by hydrogen with diameter D_2=3.21nm

Motivation

- 3D simulations are prohibited for large structures and limited to small regions. Computational intensive
- Paradigm:

"Can we use the **"Recursive"** 1D NEGF to calculate the current and density of nanostructures in which the potential has translation symmetry?"

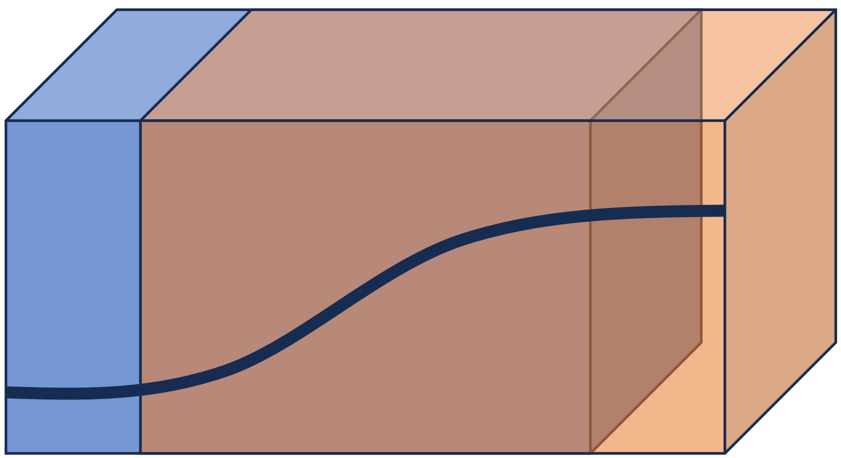
....this will require approximations

in plain words

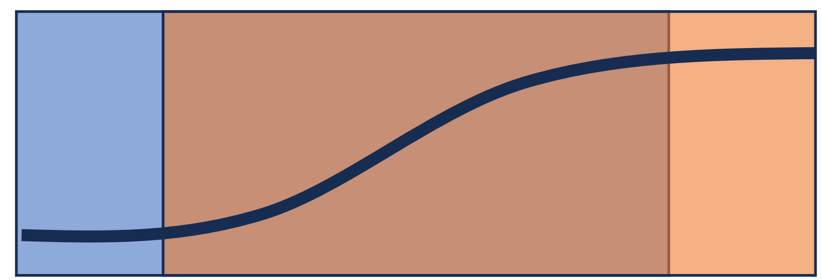
"can we use the 1D NEGF equations instead of the 3D NEGF equations?"

Motivation

"Can we just use the 1D NEGF Eqs instead of the 3D NEGF Eqs for a 3D problem with translation symmetry?"



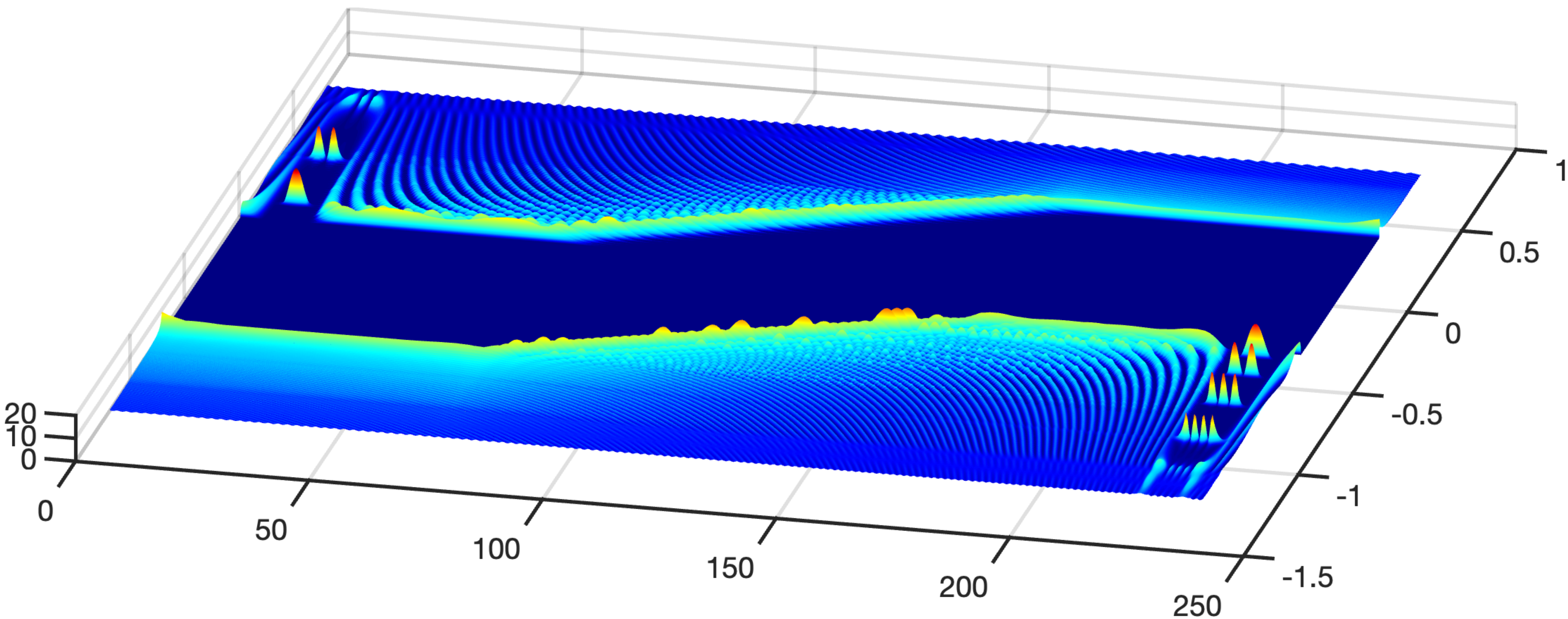
3D diode



1D diode

Motivation

- Double Barriers in Source and drain to generate hot carrier ejection means to Improve power efficiencies in solar cells, Fig. 1D DOS



M. Green (Third generation Photovoltaics, book)

Motivation

- Yes, this problem has been solved by:

PHYSICAL REVIEW B VOLUME 45, NUMBER 12 15 MARCH 1992-II

Nonequilibrium Green's-function method applied to double-barrier resonant-tunneling diodes

Roger Lake and Supriyo Datta

School of Electrical Engineering, Purdue University, West Lafayette, Indiana 47907

(Received 15 July 1991; revised manuscript received 8 November 1991)

- The problem is that they needed to calculate the complete G^R matrix, so the equations are **not suitable for the Recursive algorithm**. However, they can handle inelastic Scattering !!!

The Method(Ballistic)

The Ballistic NEGF Equations for space invariant systems:

$$\{E - E_{\perp} - H_{1D} - \Sigma_C(E - E_{\perp})\}G(E - E_{\perp}) = 1$$

$$G^{<}(E, E_{\perp}) = G\Sigma_c^{<}G^{A}$$

*Eqs (76-77) in 1964, Keldysh, "*Diagram technique for NonEquilibrium Processes*".

However, because the KMS(equilibrium) boundary condition for $\Sigma_c^{<} \sim fG$

$$G^{<}(E, E_{\perp}) = f(E)W(E - E_{\perp})$$

or

$$G^{<}(E, E_{\perp}) = \frac{f(E)}{f(E-E_{\perp})}G^{<}(E - E_{\perp}, 0)$$

Where $f(E)$ is the Fermi-Dirac function for the contact

The Method (Ballistic)

- The carrier density n_i and current j_i in point i

$$n_i = \frac{m}{2\pi^2 \Delta\, \hbar^2} \int_0^{\infty} dE \int_0^{E} dE' \, \frac{f(E)}{f(E')} \, G^{<}_{i,i}(E',0)$$

Where Δ is the spatial discretization step and $E' = E - E_{\perp}$

$$j_i = \frac{q}{\hbar \Delta^2} \int_0^{\infty} dE \int_0^{E} dE' \, \frac{f(E)}{f(E')} \left(G^{<}_{i,i+1}(E',0) - G^{<}_{i+1,i}(E',0) \right)$$

Note that the G< is current conserving for one E, then our current does not depend on the position i !!!

And that the NEGF eq in the previous slide can use the Recursive algorithm and therefore only diagonal and off diagonal elements are calculated

The Method (Ballistic)

- The previous equations can be simplified to contain one energy integration.

$$n_i = \frac{m}{\pi^2 \Delta \hbar^2} \int_0^\infty dE' \frac{\ln\left(1 + e^{-\beta(E'-\mu)}\right)}{\beta \frac{1}{1 + e^{\beta(E'-\mu)}}} G^<_{i,i}(E', 0)$$

Where μ is the fermi energy and $\beta = \frac{1}{kT}$

$$j_i = \frac{q}{\hbar \Delta^2} \int_0^\infty dE' \frac{\ln\left(1+e^{-\beta(E'-\mu)}\right)}{\beta \frac{1}{1+e^{\beta(E'-\mu)}}} \left(G^<_{i,i+1}(E', 0) - G^<_{i+1,i}(E', 0)\right)$$

Method (ballistic)

- In the case of Boltzmann statistics these expression became even simpler.

$$n_i = \frac{m}{\pi^2 \Delta\, \hbar^2 \beta} \int_0^\infty dE' G_{i,i}^{<}(E',0)$$

$$j_i = \frac{q}{\hbar \beta \Delta^2} \int_0^\infty dE' (G_{i,i+1}^{<}(E',0) - G_{i+1,i}^{<}(E',0))$$

Method (Ballistic)

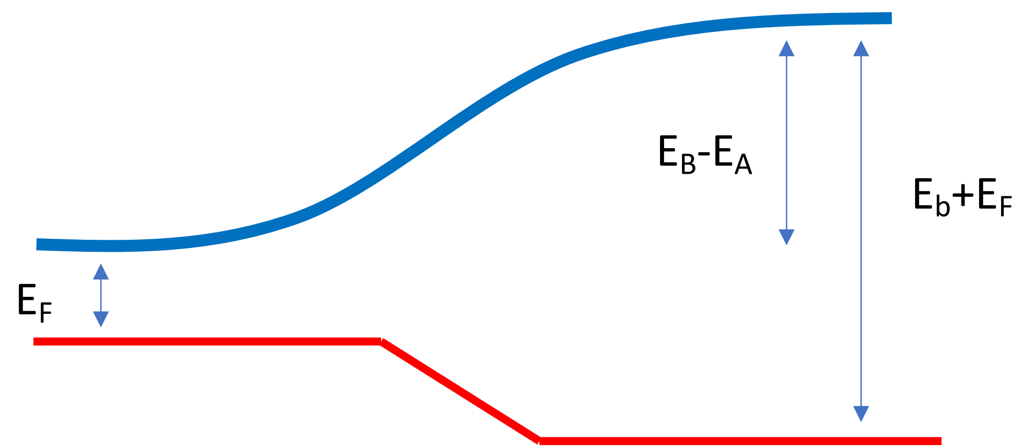
- Simple cases (Diode ballistic)

$$j = \frac{2qm}{\hbar^3 \beta^2} e^{-\beta(E_F+E_B)}(e^{\beta E_A} - 1)$$

This equation is obtained by using

$$G^< = i\ \frac{f(E) m e^{ik|z-z\prime|}}{\hbar^2 k}$$

Where $k = \sqrt{\frac{2m(E-E_\perp)}{\hbar^2}}$



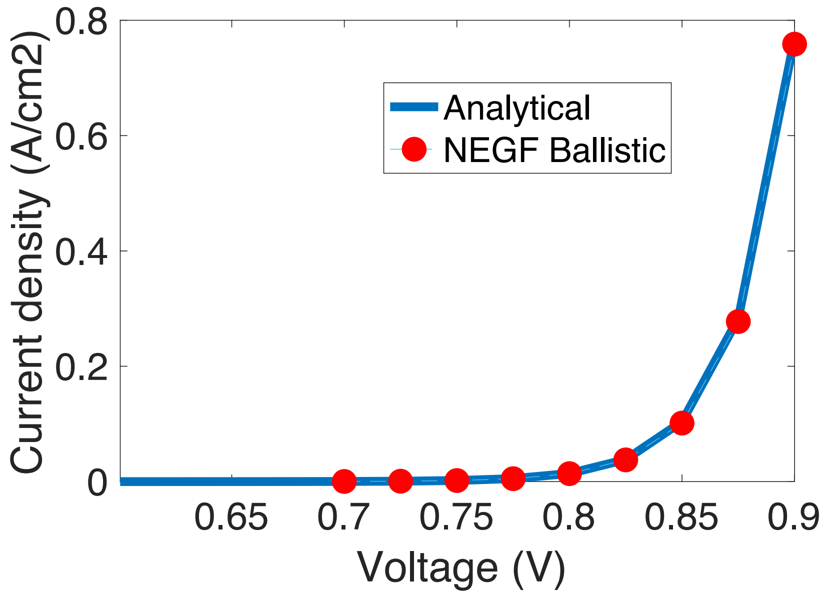
And assuming Boltzmann statistics

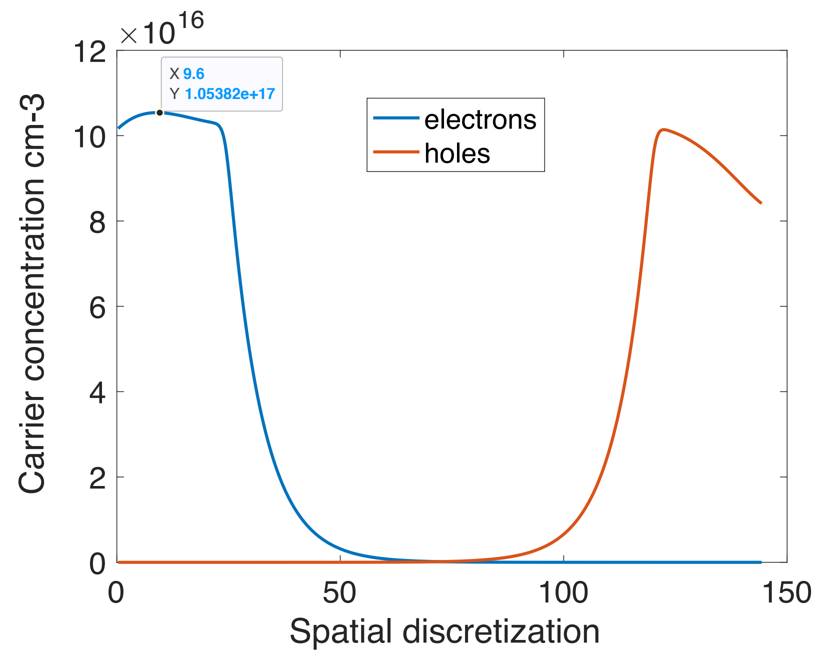
But it can also be derived from semiclassical statistical physics:

$$j = \frac{q}{4\pi^3} \iiint \frac{\hbar k_x}{m} f(\vec{k}) d^3\vec{k}$$

Ballistic Currents (GaAs)

- 1e17 in both n-i-p diode





Elastic Scattering (approximation)

$\{E - E_\perp - H_{1D} - \Sigma_C(E - E_\perp) - \Sigma_S(E - E_\perp)\}G(E - E_\perp) = 1$

$$G^<(E, E_\perp) = G(\Sigma_c^< + \Sigma_S^<)G^A$$

We assume that $\Sigma_S(E, E_\perp) = \Sigma_S(E - E_\perp)$, the self-energies need to be properly renormalized to reflect the 3D environment.

For 2 contacts:

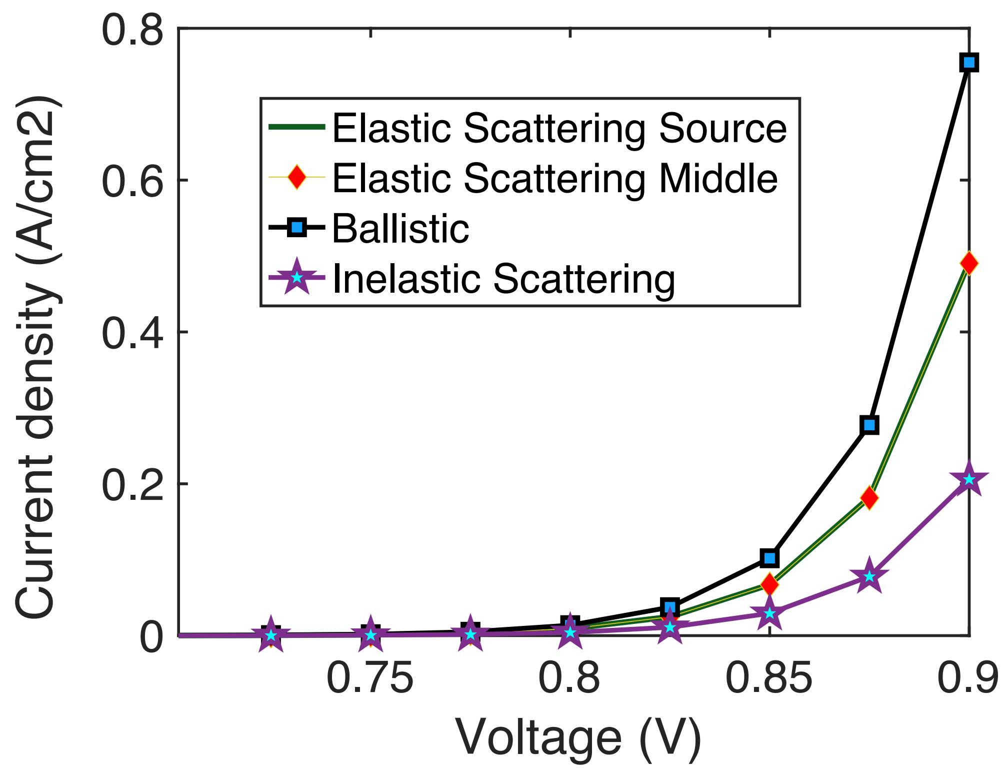
$G_1^<(E - E_\perp, 0) = G(\Sigma_1^< + \Sigma_{1S}^<)G^A$, $G_2^<(E, E_\perp) = G(\Sigma_2^< + \Sigma_{2S}^<)G^A$

$$G^<(E, E_\perp) = \frac{f1(E)}{f1(E - E_\perp)} G_1^< (E - E_\perp, 0) + \frac{f2(E)}{f2(E - E_\perp)} G_2^< (E - E_\perp, 0)$$

Note: This method is exact in the ballistic limit and does not assume that Kadanoff-Baym Ansatz ie $G^< \sim fG$, it is current conserving.

Elastic Scattering (approximation)

- GaAs pin Diode



- Current conservation elastic scattering scattering/ comparison Ballistic

Inelastic Scattering (Thoughts)

For inelastic scattering the following expression is not current conserving

(A) $$j_i = \frac{q}{\hbar\Delta^2}\int_0^\infty dE \int_0^E dE' \frac{f(E)}{f(E')}\left(G^<_{i,i+1}(E',0) - G^<_{i+1,i}(E',0)\right)$$

Let $K_i(E') = G^<_{i,i+1}(E',0) - G^<_{i+1,i}(E',0)$

For elastic scattering $K_i(E')$ is independent of i, $\Longrightarrow$ eq (A) is current conserving,

For inelastic scattering , $\int dE'\, K_i(E')$ is independent of i, so eq(A) depend on i.

For Scattering mechanism approximations :

T. Kubis'Thesis has done a wonderful work to reduce the selfenergies and study some approximations.

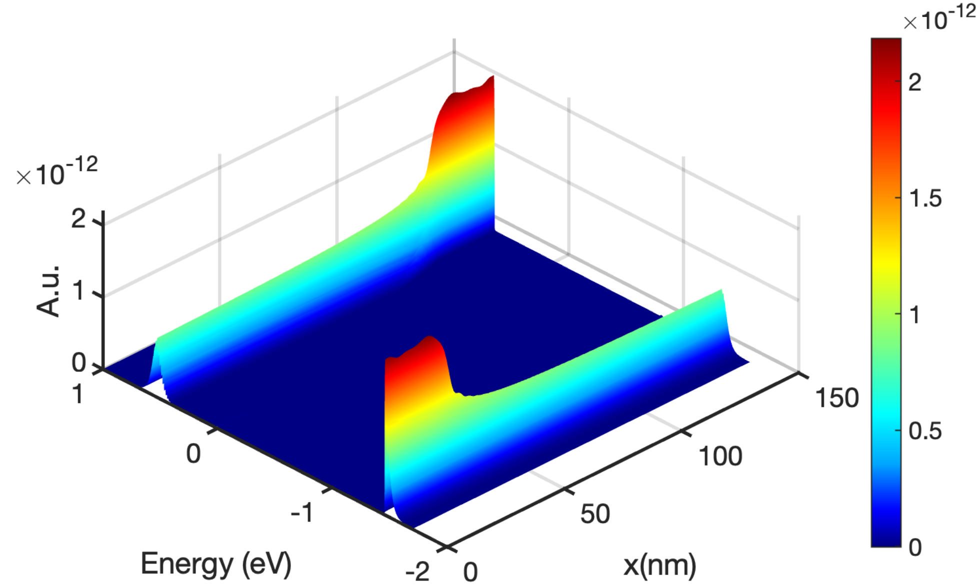
A. Svizhenko and M. P. Anantram "the role of scattering in nanotransistors", use a simple approximation

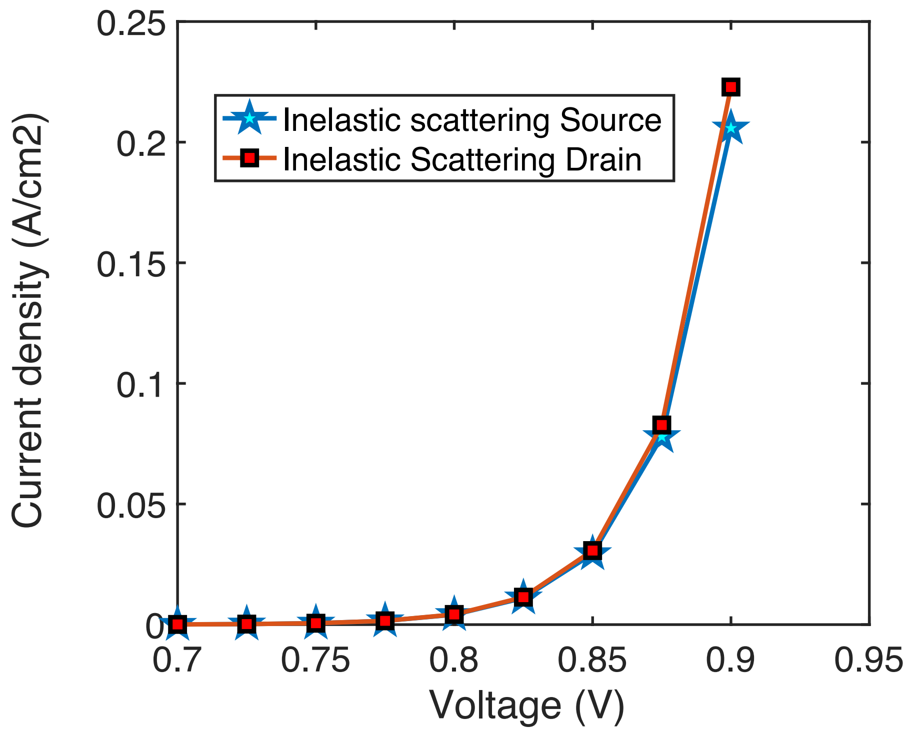
U. Aeberhard. Quantum-kinetic theory of photocurrent generation via direct and phonon-mediated optical transitions

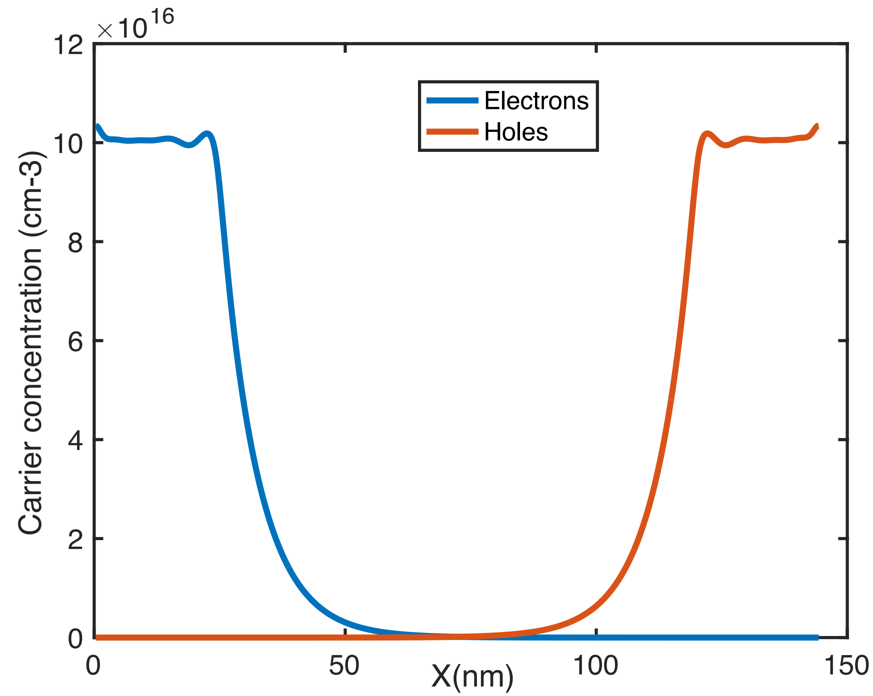
$$\Sigma^>_n(E) = \int \rho_\perp dE_\perp \sum_{q\pm} D^\pm(q)\, G^>_n\left(E \pm E_q, E_\perp\right)$$

Inelastic Scattering

- Current conservation



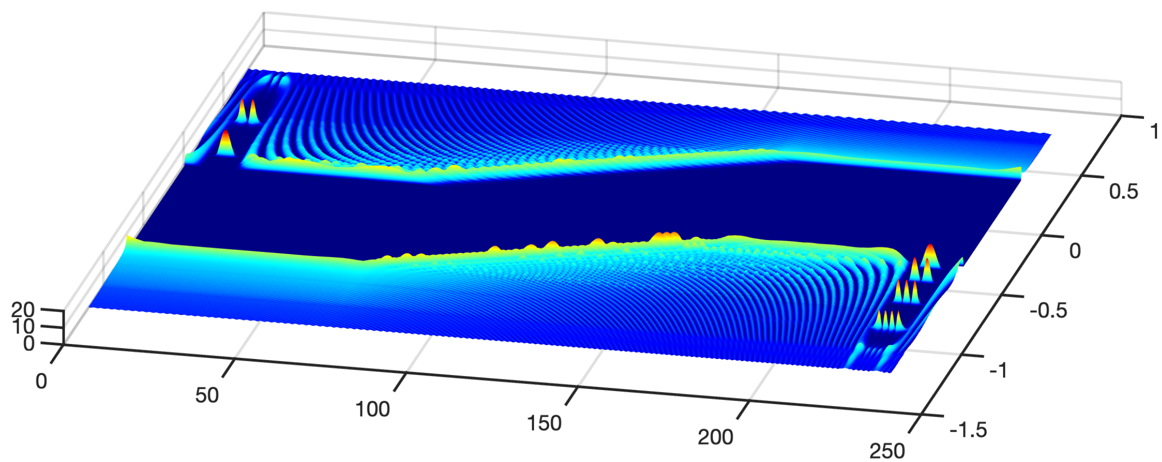




Direct Recombination

- Aims: simulation of larger structures using NEGF..length around 600nm and 20 microns wide ..for solar cell applications.
- Hot phonon descriptions…quantized injections/contacts

Example:



Density of states of a GaSb diode with resonant barriers before the end contacts. The contact material and dimension could be optimized to inject hot electron into the contacts.

Substantial work have been done by U. Aeberhard in NEGF formalism for solar cells

Direct Recombination (NEGF)

Expression for the total recombination current

$$\nabla \cdot J_n(r,E) = \frac{q}{2\pi\hbar} \int dr' (G_n^{<} \Sigma_n^{>}(E) - G_n^{>} \Sigma_n^{<}(E))$$

Emission Absorption

$$I = \frac{q}{2\pi\hbar} \int dr \int dE \int dr' (G_n^{<} \Sigma_n^{>}(E) - G_n^{>} \Sigma_n^{<}(E)) \quad (1)$$

$$I = q n_i^2 B\, V\, (e^{\beta E_{ap}} - 1) \quad (2)$$

- B Roosbroeck constant, n_i intrinsic concentration, V volume. No photon recycling considered.

*M. Green (Photovoltaics) and W. van Roosbroeck and W. Shockley (Phys. Rev. 94, 1558 (1954)). Shockley-Queisser, Journal of Applied Physics. **32** (3): 510–519*

Direct Recombination (NEGF)

The self-energy for electron-hole recombination (outscattering)

$$\Sigma_n^{>}(E) = \sum_q M(q)(N_q+1)G_p^{<}(E - E_q)$$

Nq= Bose-Einstein distribution, M(q) coupling constant.

$$\Sigma_n^{>}(E) = D^* \, G_p^{<}(E - E_G^*)$$

- D* is a renormalized coupling. E_G* (slightly larger than the Bandgap) is between the maximum of *n(E)* and *p(E)*.
- We can find the constant D* by putting Eq (1)=Eq (2) for generation

Even if photon Absorption and Emission are inelastic processes, the electron-hole system is current conserving at each energy.

Conclusions

- An exact method to solve 3D NEGF by solving 1D NEGF for **Ballistic** for Translation invariant systems (TI).
- For **Elastic Scattering**, an approximate method to solve 3D NEGF by 1D NEGF
- For a **Restricted Recombination model**, 3D NEGF can be substituted by 1D NEGF
- For **Inelastic Scattering** the method is not current conserving and needs to be modified, however in most of the cases, the error in current conservation is good enough.

References. (thanks for your attention)

R. Lake and S. Datta, Nonequilibrium Green's-function method applied to double-barrier resonant-tunneling diodes" *Phys. Rev. B 45, 6670 (1992).*

U. Aeberhard. "Challenges in the NEGF Simulation of Quantum-Well Photovoltaics Posed by Non-Locality and Localization." Physica status solidi (b) 256 (2019), (see other references from author).

- A. Svizhenko and M. P. Anantram, "Role of scattering in nanotransistors," in *IEEE Transactions on Electron Devices*, vol. 50, 6, pp. 1459-1466, (2003),
- T. C. Kubis, "*Quantum transport in semiconductor nanostructures*", (2009)