COMPUTATIONAL ASPECTS OF SOLID STATE TRANSPORT

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INTRODUCTION

Overview over computational techniques for charged carrier transport in solid state materials in intermediate regimes.

- 3 Generations of solar cells, varying in size (thin films) and technology (heterojunctions).
- Compromise between first principle modeling and actual device simulation $\Rightarrow$ bridge multiple scales in modeling.
- Focus on two problem areas: Methods for stiff transport systems and interaction with barriers.

Issues

- 'Larger' mean free path (compared to device size, 2G, thin films) $\Rightarrow$ non - Maxwellian effects $\Rightarrow$ kinetic theory.
- Heterojunctions (3G): multiple materials; generate potential barriers due to jumps in the bandgap; band structure.
- Quantum effects: Present below $50 - 100nm$ length scales at potential barriers.

Model equations $_{02}$

1. Semi - classical: Boltzmann equation for electrons and holes. Collisions: mainly electron - phonon; Generation / Recombination: Auger, SRH, Excitation by Photons.
2. Quantum effects: Schrödinger, Wigner, density matrices, Green's functions. Transport not purely ballistic (temperature effects etc.) $\Rightarrow$ mixed classical - quantum models.

OUTLINE $_{03}$

- Deterministic methods for systems of Boltzmann equations as an alternative to Monte Carlo.
  - Multiple time scales, steady state calculations.
  - Discretization methods, difference vs. spectral.
- Quantum mechanical interactions with potential barriers in otherwise classical simulations.
  - Effective energy approaches in semiclassical Monte Carlo codes.
  - Higher dimensional scattering matrix approaches.

PART I: Deterministic methods for the BTE $_{05}$

$$\partial_t f^{(\nu)} + \nabla_x \cdot (f^{(\nu)} \nabla_p \mathcal{E}^{(\nu)}) - \nabla_p \cdot (f^{(\nu)} \nabla_x \mathcal{E}^{(\nu)}) = Q[f^{(\nu)}] + \nu R$$

$$\mathcal{E}^{(\nu)}(x,p) = B(p) + \nu V(x), \quad \nu = \pm 1$$

$f^{(\nu)}(x,p,t)$: kinetic density, $\nu = \pm 1$: electrons and holes.

V : Potential, computed from Poisson equation.

$B(p)$: kinetic energy from the band diagram.

Q: collisions with lattice vibrations (phonons).

R: Generation / recombination (Recombination can happen on a much larger time scale.)

Collisions: Fermi's Golden Rule

- High temperature: dominant mechanism = scattering with lattice vibrations (phonons) $\Rightarrow$ linear.
- FGR: Scattering with the lattice results in a change of energy of $\pm\hbar\omega$ $\Rightarrow$ sparse in energy.

$$Q[f^{(\nu)}](x,p,t) = \int K(p,q) f^{(\nu)}(x,q,t) - K(q,p) f^{(\nu)}(x,q,t)\, dq$$

$$\boxed{K(p,q) = \sum_{\sigma=\pm 1} s_\sigma(p,q)\delta(B(p) - B(q) + \sigma\hbar\omega)}$$

Expansion methods $_{06}$

Expand the density function $f^{(\nu)}$ in basis function of the kinetic energy B of the electron and the momentum direction κ.

$$p = |p|\kappa,\ \kappa \in \mathcal{S}_3,\ |\kappa| = 1,$$

$$\boxed{f^{(\nu)}(x,p,t) \approx \sum_{n=1}^{N} f_n^{(\nu)}(x, B(p), t) S_n(\kappa)}$$

$S_n(\kappa)$: Spherical harmonics.

Advantage: Fermi's Golden Rule ($Q \approx \delta(B(p) - B(q) \pm \hbar\omega)$) becomes a difference operator in the new variable $e = B(p)$.

A hyperbolic system in (x, e) for the expansion coefficients

$$\partial_t f_n^{(\nu)} + \sum_m \nabla_x \cdot [a_{nm} f_m^{(\nu)}] - \nu \nabla_x V \cdot [b_{nm} + c_{nm} \partial_e] f_m^{(\nu)} = [\mathbf{Q} f^{(\nu)}]_n + \nu R_n$$

for the expansion coefficients $\boxed{f_n^{(\nu)}(x, e, t),\ e = B(p)}$.

Advantages:

1. $\mathbf{Q}$ is sparse and easily inverted $\Rightarrow$ deal with stiffness using partially implicit methods. Compute steady states directly.

2. Use symmetries of the geometry for $x \in \mathbb{R}^2$ and $x \in \mathbb{R}^1$ simulations.

3. The hyperbolic system retains the same entropy properties as the original Boltzmann equation.

Entropy

The relative entropy

$$\boxed{-\int f(\ln f + \mathcal{E})\, dx dp}$$

for the resulting hyperbolic system increases

$\Rightarrow$ stability for the hyperbolic system

Approaches (1)$_{09}$

Discretizing the energy $e = B(p)$:

- Same as the spatial discretization $\Rightarrow$ yields a positive operator (and guarantees positive densities).
- Spectral discretization of the energy using Hermite functions (in general: polynomials $\times$ equilibrium distribution).

$$\boxed{f_n^{(\nu)}(x,e) = \sum_k f_{nk}^{(\nu)}(x) P_k(e) \exp(-e)}$$

cheaper, but limited in highly non - equilibrium regimes.

Approaches (2)

Transient vs. steady state

- Transient: Use hyperbolic methods for hyperbolic systems (WENO or DG, Carrillo, Gamba, Majorana, Shu).
- Steady state: Elliptic solvers in a weighted L^2 space and Hermite polynomials in energy. (Heitzinger, Vasileska, CR), reduces to standard discretization for dteady state drift - diffusion if only one basis function is taken.

Simulation of an MOS-transistor

Electron density and energy; potential and lateral current component.

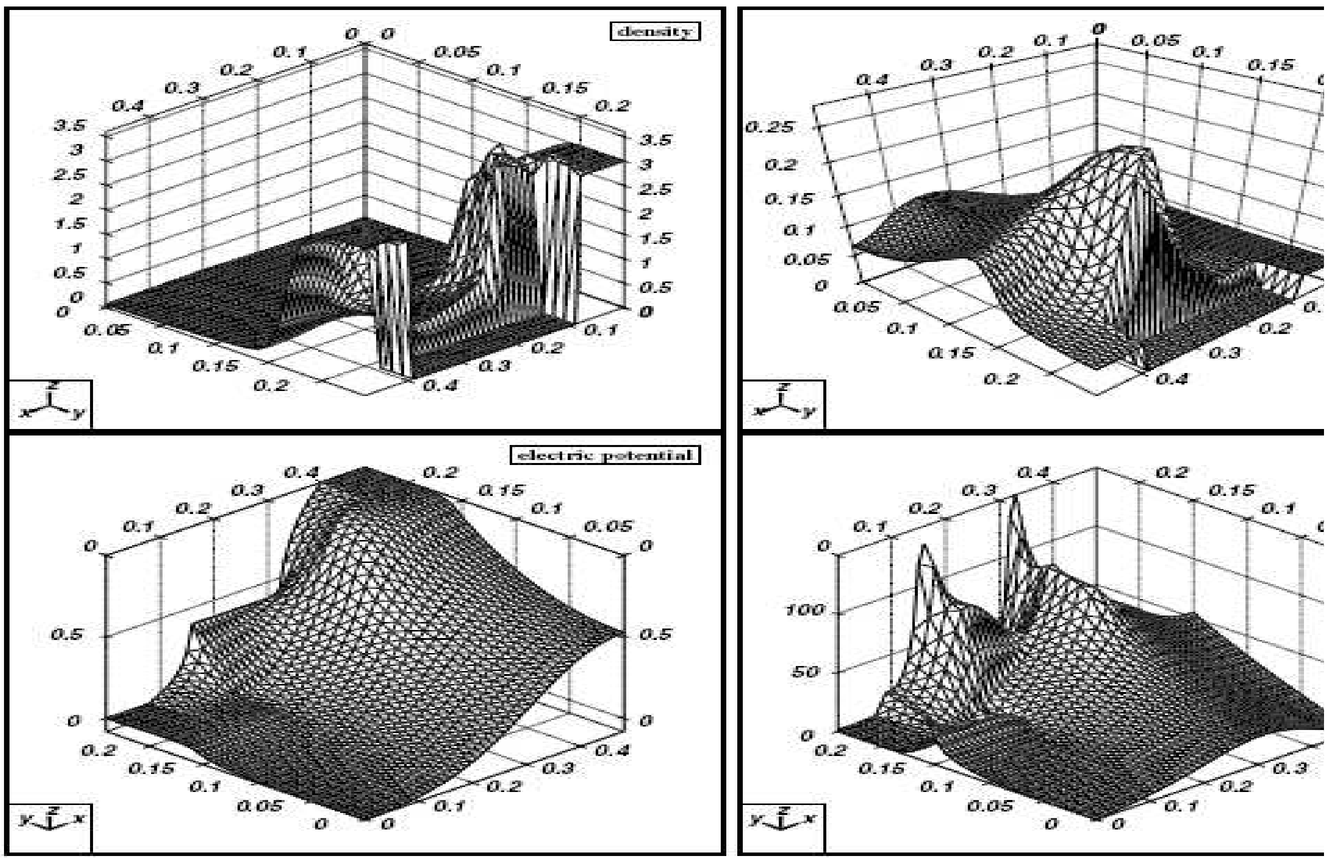


Fig. 11. MOSFET device. BTE results. $t = 5$ ps. Top left: the charge density ρ (10^{-17} cm^{-3}); top right: the energy $\mathscr{E}$ (eV

Non - Maxwellian effects

Moment distribution of the kinetic density at various points of real space

$x_1 = 50nm,\ f(50, p_1, p_{23})B(p)$.

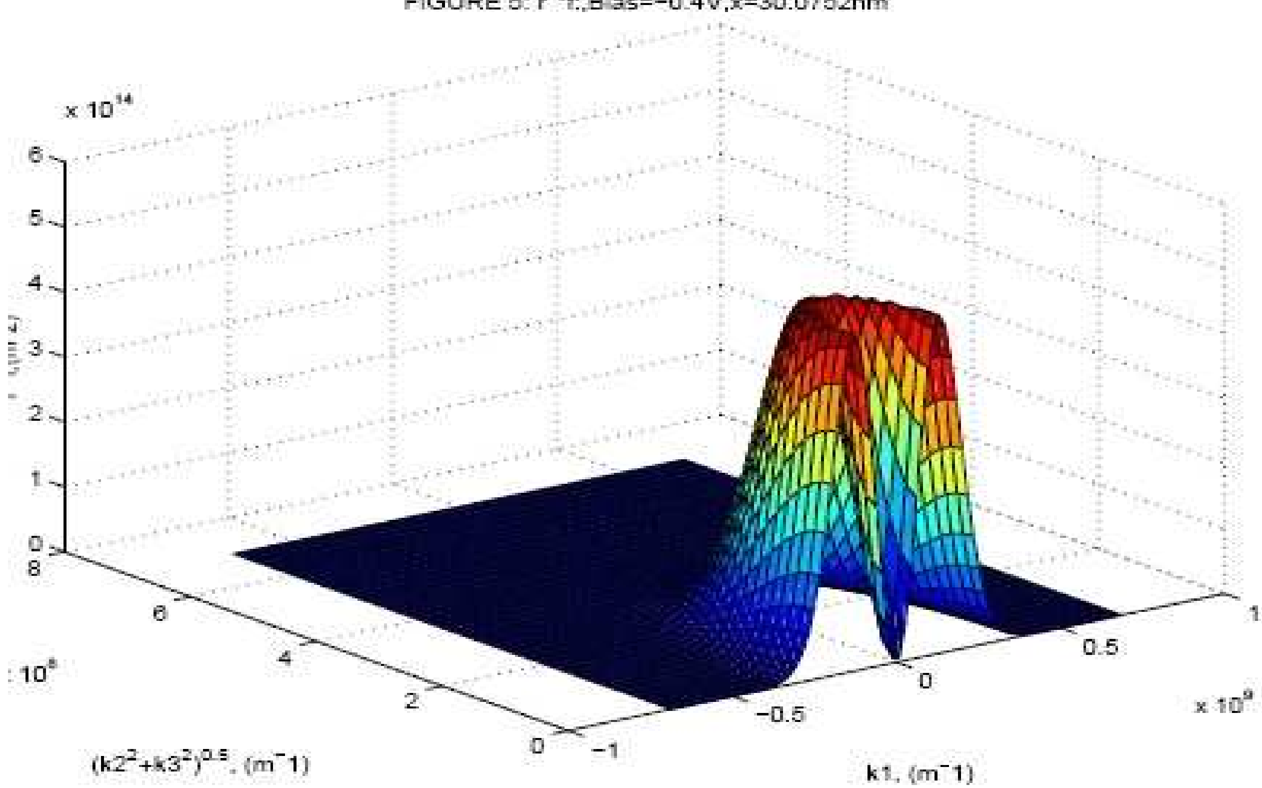
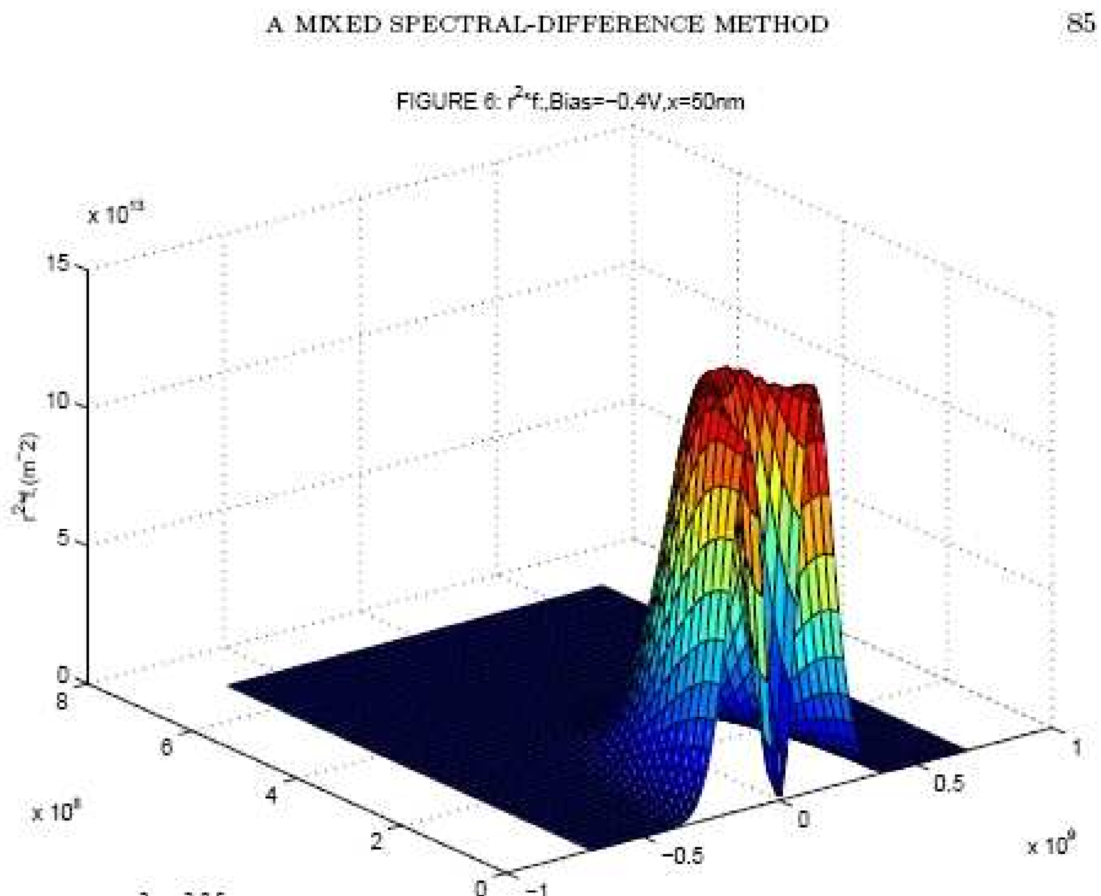


FIG. 5. $r^2 * f$: $Bias = -0.4V$, $x = 30.0752nm$.

Non - Maxwellian effects

Moment distribution of the kinetic density at various points of real space $x_1 = 100nm\ f(100, p_1, p_{23})B(p)$.



Non - Maxwellian effects

Moment distribution of the kinetic density at various points of real space $x_1 = 150nm\ f(150, p_1, p_{23})B(p)$.

FIGURE 7: r^2*f, Bias=−0.4V,x=100nm

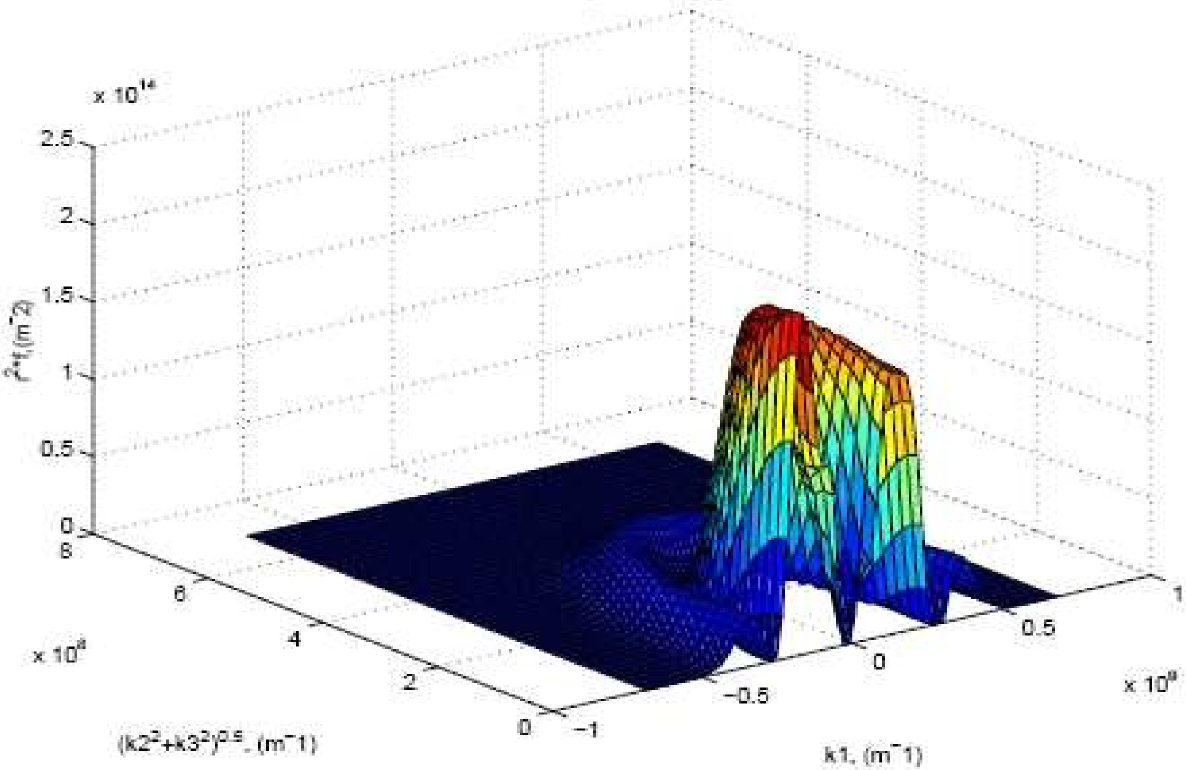


Fig. 7. $r^2 * f$: $Bias = -0.4V$, $x = 100nm$.

Summary

- Expansion methods are practical for $x \in \mathbb{R}^2$. (3D possible but is HPC).
- Superior to MC in 2D if stiffness (generation / recombination) is included and steady states are needed.
- Easy to couple with Poisson, but cannot include many body theory beyond mean fields.

PART II: Approximate quantum mechanics $_{12}$

Goal: Include q.m. transport mechanisms approximately into an otherwise classical simulation.

- Interaction with barriers caused by jumps in bandgaps from one material to another in heterojunction devices.
- Heterojunction devices: MESFET, tunneling diodes, 3G solar cells.

The Wigner Boltzmann equation $_{13}$

Equivalent to the Heisenberg equation for the density matrix of a mixed state (after Fourier transform).

$$\boxed{f(x,p,t) = \mathcal{W}\rho(x,p,t) = \int \rho(x - \tfrac{\hbar}{2}\eta, x + \tfrac{\hbar}{2}\eta, t) e^{i\eta\cdot p}\, d\eta}$$

$$\partial_t f^{(\nu)} + \mathcal{C}_W\{\mathcal{E}^{(\nu)}, f^{(\nu)}\} - \nabla_p \cdot (f^{(\nu)} \nabla_x \mathcal{E}^{(\nu)}) = Q[f^{(\nu)}] + \nu R$$

$$\boxed{\mathcal{C}_W\{\mathcal{E}^{(\nu)}, f^{(\nu)}\} = \tfrac{i}{\hbar} \textstyle\sum_{\sigma=\pm 1} \sigma \mathcal{E}^{(\nu)}(x - \tfrac{i\sigma\hbar}{2}\nabla_p, p + \tfrac{i\sigma\hbar}{2}\nabla_x) f^{(\nu)}}$$

$\mathcal{C}_\mathcal{W}$ converges in the limit $\hbar \longrightarrow 0$ to the classical commutator

$$\boxed{\mathcal{C}_c = \nabla_p \mathcal{E}^{(\nu)} \cdot \nabla_x f^{(\nu)} - \nabla_x \mathcal{E}^{(\nu)} \cdot \nabla_p f^{(\nu)}.}$$

Problems:

- There is no first principle formulation for Q, other than oscillator bath. (Scattering on the qm level only given in a Green's function formulation.)
- The quantum commutator $\mathcal{C}_W$ is a pseudo differential operator whose kernel is not uniformly positive. ($\Rightarrow$ negative particles because of violation of the Heisenberg principle $\Rightarrow$ geometric explosion).
- Particles allow us to go beyond mean field theory.

2 approaches to model interaction with potential barriers rudimentarily on a q.m. level.

Approach 1 : Effective energies$_{15}$

Idea: Replace the action of the potential V on the particle by the action of an effective potential, which produces the same result in local thermal equilibrium.

Local thermodynamic equilibrium:

- Zwanzig, Degond, Mehats, CR: Generalization of Levermore closures in the classical case.
- Local equilibrium defined as the maximizer of the entropy under the constraint of a given observation.

The relative Von Neumann entropy for the density matrix of a mixed state

$$S[\rho] = -Trace[\rho \cdot (\ln(\rho) + H - id)], \quad H = -\frac{\hbar}{2m}\Delta_x + V$$

The local thermal equilibrium $f_{equ}^{(n)} = \mathcal{W}\rho_{equ}^{(n)}$

Given by the constrained optimization problem

$$\boxed{S[\rho_{equ}^{(n)}] = \max\{S[\rho] : \ \rho(x,x) = n(x)\}, \quad n(x) = \int f(x,p)\, dp}$$

$\rho_{equ}^{(n)}$ given in terms of an operator exponential and a Lagrange multiplier λ

$$\boxed{\rho_{equ}^{(n)}(x,y) = \mathcal{E}xp[-\mathcal{E}(i\hbar(\nabla_x - \nabla_y))\delta(x-y) - \lambda(x)\delta(x-y)]}$$

$$f_{equ}^{(n)} = \mathcal{W}[\rho_{equ}^{(n)}] = e^{\mathcal{E}_{eff}(x,p)}$$

Algorithm $_{18}$

(1) Given $f(x,p,t) = \sum_k \delta(x - x_k)\delta(p - p_k)$

(2) Compute $n(x,t) = \int f(x,p,t)\, dp$ on a mesh by a cloud in cell method.

(3) Compute $f_{equ}^{loc} = f_{equ}^{loc}(n)$: the entropy minimizer for the particle density $n(x,t)$.

$$\rho_{equ}^{loc}(x,y,t) = \exp[-\Delta\delta(x-y) - \lambda(x)\delta(x-y)]$$

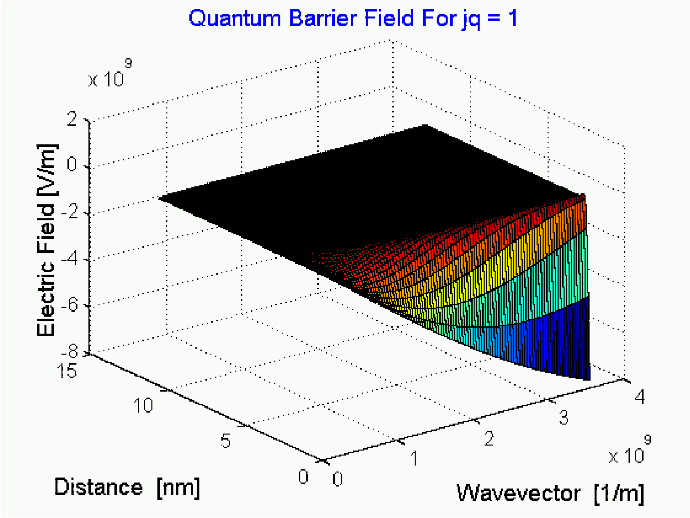
$$\boxed{\lambda : \ \rho_{equ}^{loc}(x,x,t) = n(x,t)}$$

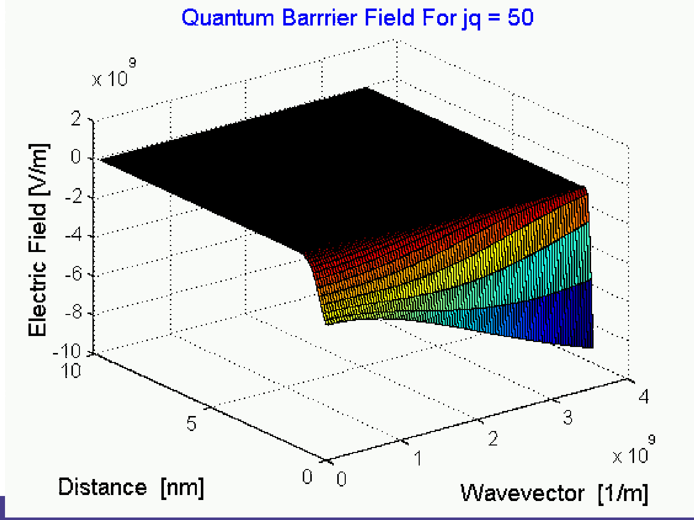
(4) Compute the effective energy $\boxed{\mathcal{E}_{eff} = \frac{\mathcal{E}_q(x,p,\nabla_x,\nabla_p) f_{equ}^{loc}}{f_{equ}^{loc}}}$

(5) Move the particles according to the classical commutator with $\mathcal{E}_{eff}$.

(6) Scatter according to classical collision operator.

Effective force for a step





The resulting potential (or field) is dependent on the wave vector p!

Quantum corrected force for a step potential as a function of distance and wave vector

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low cross directional energy

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high cross directional energy

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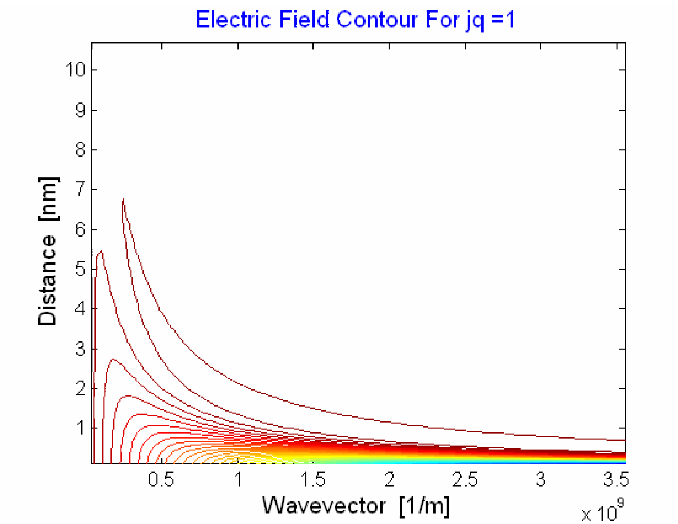
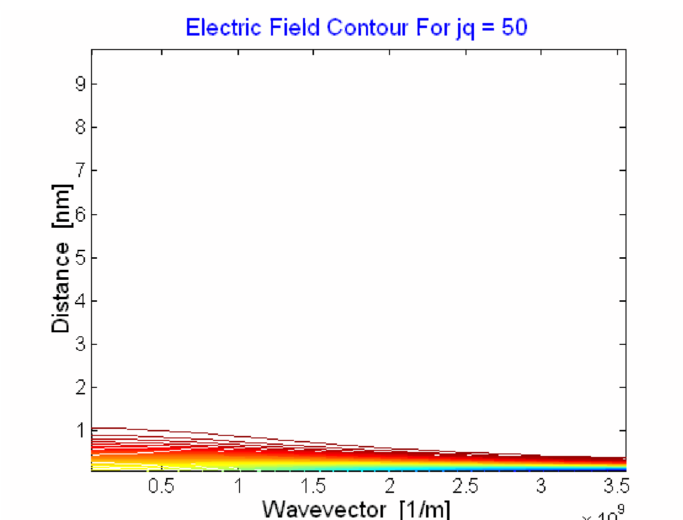
Contours





High energy particles behave more classically.

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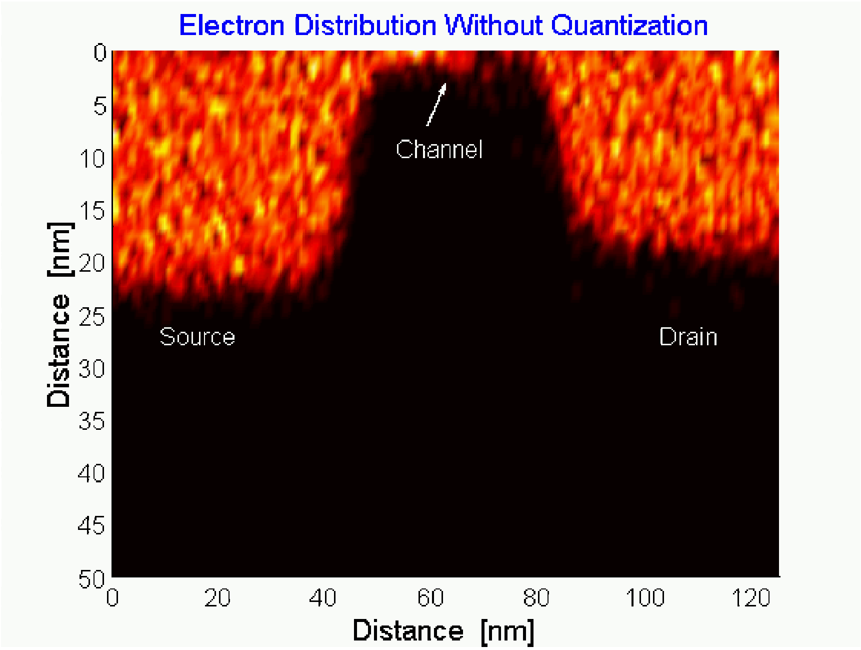
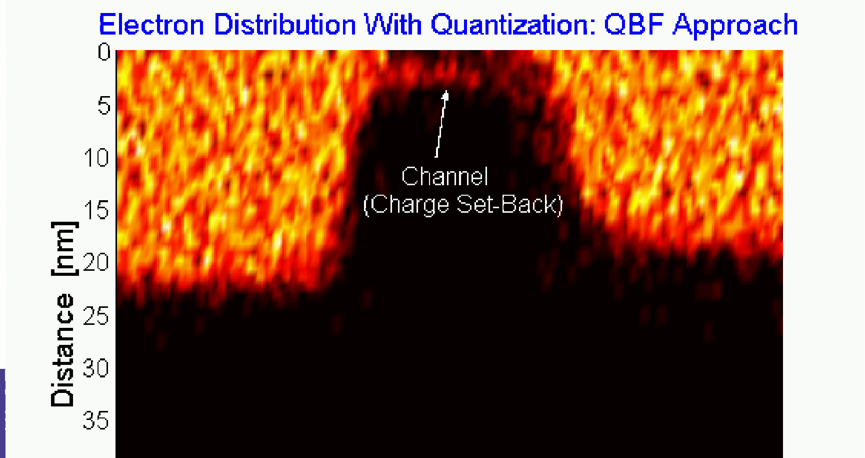
Charge Separation from the gate in a 20nm MOSFET





Particles move along the barrier at a distance due to the nonlocal interaction with the barrier -

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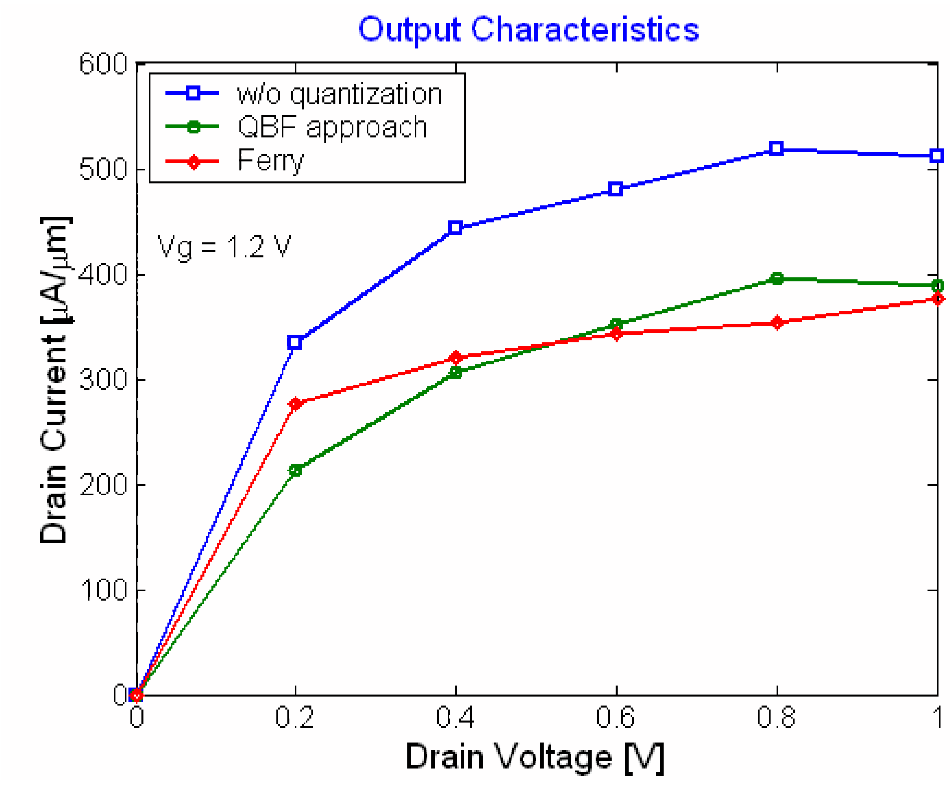
Current vs. Voltage



This reduces the output significantly

Approach 2: Generalization of scattering matrix approaches$_{20}$:

Idea: Use classical transport picture away from barriers.

$$\frac{dx}{dt} = \frac{p}{m}$$

Compute the probability of transmission / reflection by the barrier by solving a 1-D scattering problem for the Schrödinger equation exactly in the direction orthogonal to the barrier.

$$\boxed{i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\partial_x^2\psi + V\psi, \quad V(x) = \begin{pmatrix} V_- & for & x<0 \\ V_+ & for & x>0 \end{pmatrix}}$$

$$\psi(x,t) = \begin{pmatrix} \exp(i\frac{xp_-}{\hbar} - i\omega t) + R\exp(-i\frac{xp_-}{\hbar} - i\omega t) & for & x < 0 \\ T\exp(i\frac{xp_+}{\hbar} - i\omega t) & for & x > 0 \end{pmatrix}$$

$$\boxed{p_+ = \sqrt{p_-^2 - m\Delta V}}$$

For $p_-^2 < m\Delta V$ this gives an evanescent transmitted wave, which is neglected in the semiclassical approximation.

$$T = \begin{pmatrix} \frac{2p_-}{p_- + p_+} & for & p_-^2 > m\Delta V \\ 0 & for & p_-^2 < m\Delta V \end{pmatrix}, \quad R = \begin{pmatrix} \frac{1-p_+}{p_- + p_+} & for & p_-^2 > m\Delta V \\ 1 & for & p_-^2 < m\Delta V \end{pmatrix}$$

In higher dimensions (Jin, Novak '04)

The reflection / transmission coefficients and the transmitted momentum direction p_+ depend also on the angle the wave impacts the interface. write p_- as

$$\boxed{p_- = \alpha_- \mathfrak{N} + \beta_- \mathfrak{T}, \quad p_+ = \alpha_+ \mathfrak{N} + \beta_+ \mathfrak{T},}$$

$$\boxed{\alpha_+^2 + \beta_+^2 = \alpha_-^2 + \beta_-^2 - m\Delta V}$$

with $\alpha_- = \mathfrak{N} \cdot p_-$ and $\beta_- = \mathfrak{T} \cdot p_-$.

($\mathfrak{N}, \mathfrak{T}$: normal and tangent vector to the barrier.)

Yields $R(\alpha_-, \beta_-)$ and $T(\alpha_-, \beta_-)$ and $\beta_+(\alpha_-, \beta_-)$

Algorithm $_{24}$

Solve Newton equations for one time step

$$\boxed{\tilde{x}(t+\Delta t) = x(t) + \frac{\Delta t}{m} p(t)}$$

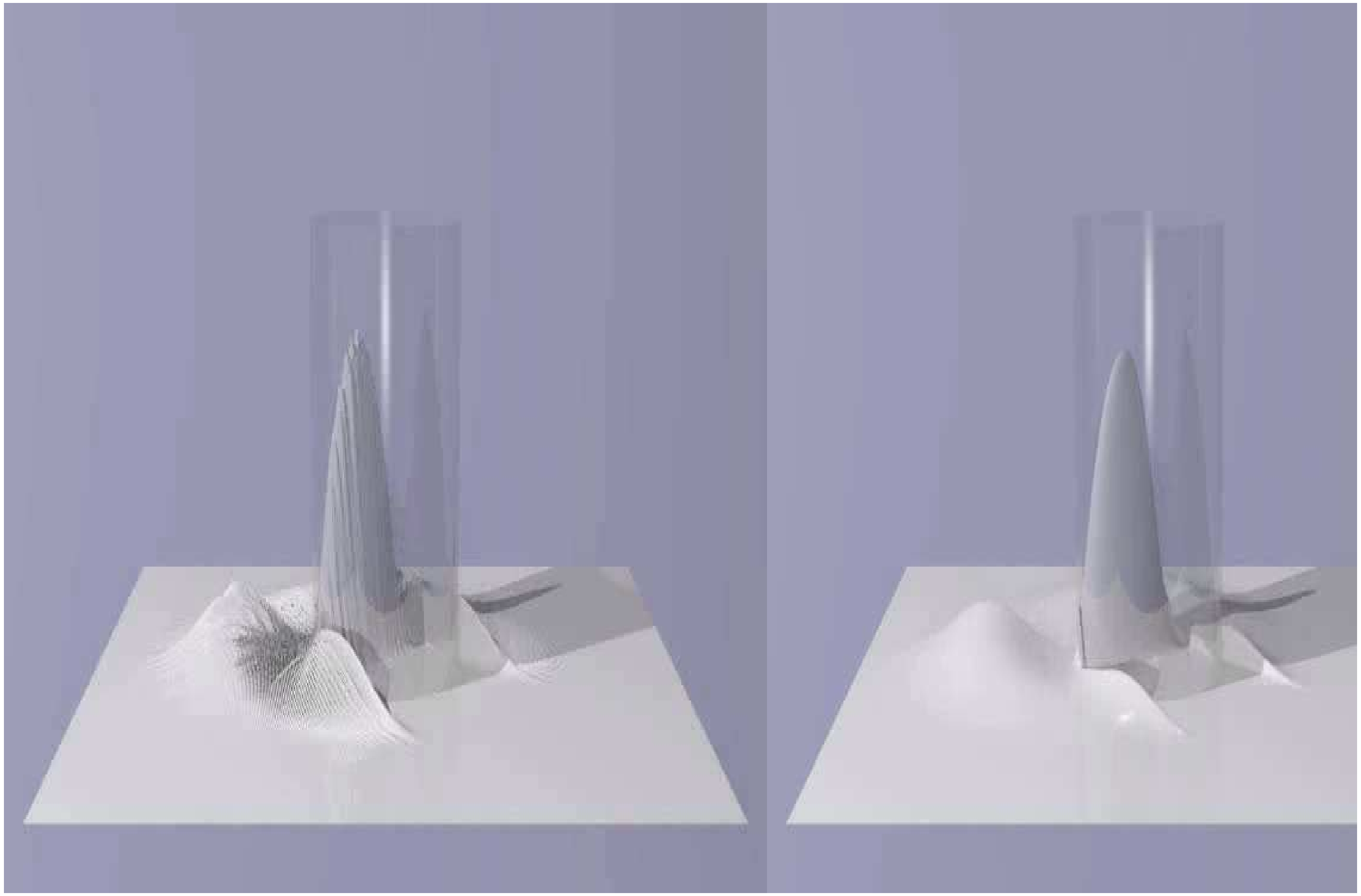
If $\tilde{x}$ has crossed a barrier: $p(t) = \alpha_- \mathfrak{N} + \beta_- \mathfrak{T}$

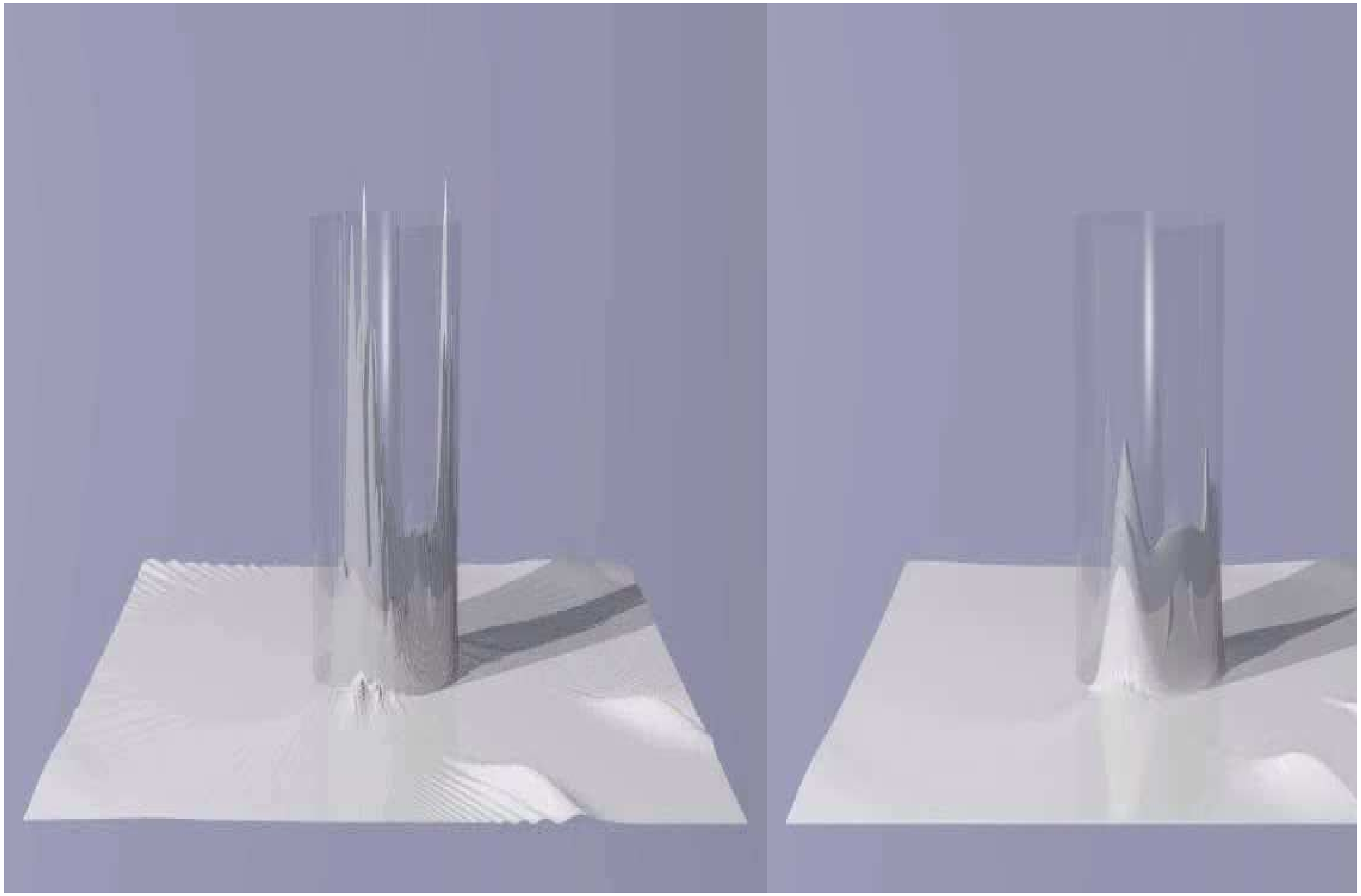
$$x(t+\Delta t) = \begin{pmatrix} \tilde{x}(t) & \text{with probability } T \\ x(t) & \text{with probability } R \end{pmatrix}$$

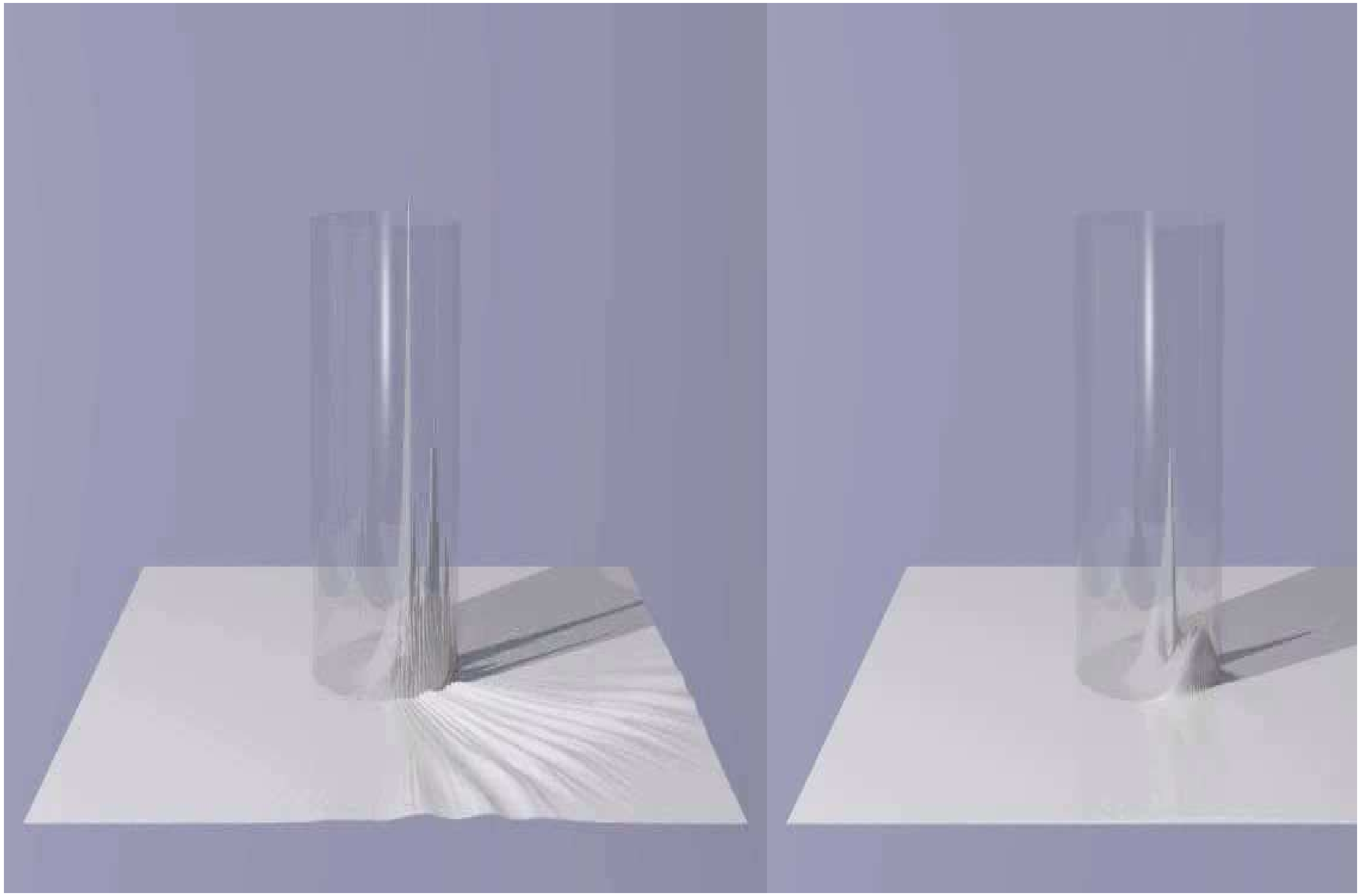
$$p(t+\Delta t) = \begin{pmatrix} p(t) & \text{with probability } T \\ -\alpha_- \mathfrak{N} + \beta_+ \mathfrak{T} & \text{with probability } R \end{pmatrix}$$

T, R, β_+ depend on α_-, β_-!

Example: Semiclassical ballistic scattering at a 'semiclassical' glass







Conclusions $_{26}$

- Tools for simulation of charged particle transport in solids.
- Applicability to 2G - 4G solar cells.
  - Vastly different time scales (collisions vs. generation)
  - Barriers
- Many body problems beyond mean fields using particle based methods and P^3M and FMM approaches.
- Stochasticity due to random (unintentional) dopants .