SUB-BAND MODELING OF TRANSPORT IN NARROW GEOMETRIES

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JOINT WORK WITH

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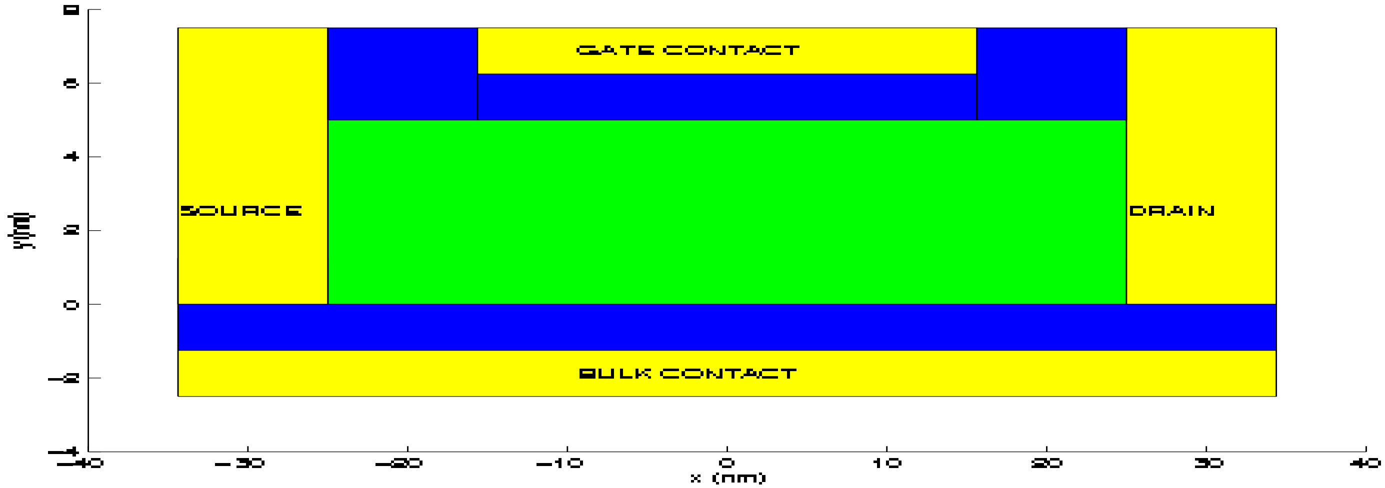
INTRODUCTION

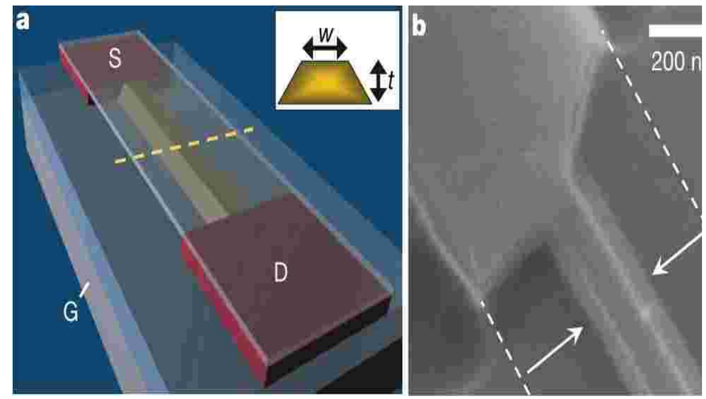
- Charged particle transport in confined geometries
- Thin films and narrow tubes (channels).
- Goal: Models that allow for simulation on long time scales.

APPLICATIONS 1

Thin films:

Nano-scale logics and analog devices. SOI (Silicon on Insulator) technology. Solar cells.





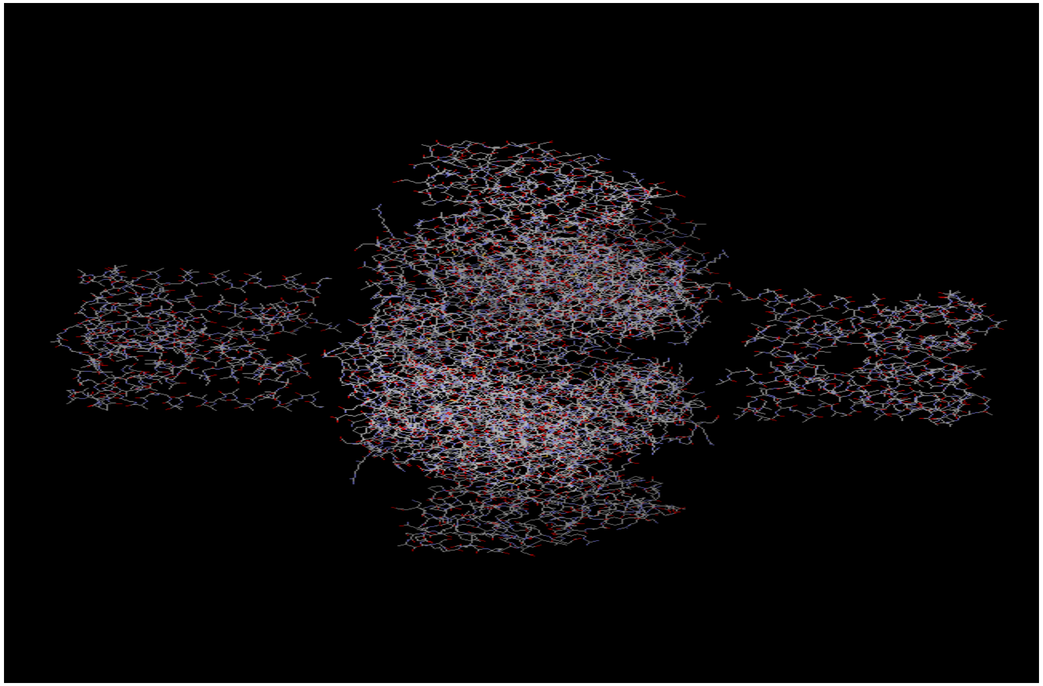
Modulate the current through very small variations in the gate voltages.

APPLICATIONS 2

Thin tubes: Proteins and Ion channels

Transport of charged molecules (ions) in water and in complicated geometries.

Protein 1LNQ



The Transport Picture $_{05}$

Hamiltonian dynamics + collisions with a background

confined geometries.

Model hierarchy :

1. Molecular Dynamics. (compute the background).
2. Monte Carlo. (collisions with random background).
3. Kinetic equations for phase space densities.
4. Macroscopic models (Hydrodynamics, Diffusion etc.)

1-3: physical transport mechanisms.

4: function of the structure on large time scales.

KINETIC MODELS$_{07}$

$$\partial_t f + \{\mathcal{E}, f\} = Q[f], \quad \mathcal{E}(X,P) = V(X) + \frac{|P|^2}{2}$$

$f(X,P,t)$: phase space density (X:space, P: momentum)

$\{\mathcal{E}, f\}$: Hamilton operator (Poisson - bracket, ballistic transport)

Classical picture: Newton equations $\frac{dX}{dt} = P,\ \frac{dP}{dt} = -\nabla_X \mathcal{E}$

$$\{\mathcal{E}, f\} = \nabla_X \cdot (\nabla_P \mathcal{E} f) - \nabla_P \cdot (\nabla_X \mathcal{E} f)$$

Quantum picture via Wigner functions (Pseudodifferentialoperators):

$$\{\mathcal{E}, f\} =$$

$$\frac{1}{2}\int_{-1}^{1} \nabla_X \cdot [\nabla_P \mathcal{E}(X, P + \frac{s\hbar}{2i}\nabla_X) f] - \nabla_P \cdot [\nabla_X \mathcal{E}(X - \frac{s\hbar}{2i}\nabla_P, P) f]\, ds$$

Collisions

$$\boxed{\partial_t f + \{\mathcal{E}, f\} = Q[f]}$$

Q:Dissipative collision operator (scattering with the background)

Boltzmann: Integraloperator

$$\boxed{Q[f](X,P) = \int S(f,P,P')f(X,P') - S(f,P',P)f(X,P)\,dP'}$$

Fokker-Planck (Wiener process, random walk)

$$\boxed{Q[f](X,P) = \nabla_P \cdot [\nabla_P f + \gamma P f]}$$

Q relaxes against some notion of thermodynamic equilibrium $\Rightarrow$ large time asymtotics.

OUTLINE$_{11}$

- Part 1: General principles
  - Confined geometries, anisotropic energy dissipation $\longrightarrow$ fluid models with free energy variables.
- Part 2: Classical transport in narrow channels.
  - Computational complexity. Locally harmonic potential approximation. Numerics.
- Part 3: Quantum transport in thin films.
  - Conservation laws and local entropies.

CONFINED GEOMETRIES$_{13}$

$$\boxed{X = (x, y) \in \Omega = \Omega_x \times \Omega_y \text{ with } |\Omega_y| << |\Omega_x|}$$

x: transport direction, y: confinement direction.

$$P = (p, q)$$

- Thin films : $x, p \in \mathbb{R}^2,\ y, q \in \mathbb{R}^1$
- Narrow channels: $x, p \in \mathbb{R}^1,\ y, q \in \mathbb{R}^2$

SCALES$_{14}$

$y << x \rightarrow y = O(\varepsilon)$

ε: aspect ratio

Rescale:

$$y \longrightarrow \frac{y}{\varepsilon}, \quad q \longrightarrow \frac{q}{\sqrt{\varepsilon}}, \quad t \longrightarrow \frac{t}{\varepsilon}$$

Principle:

- A collision with the background in the confinement direction y is a rare event compared to collisions with the background in the transport direction x.
- Energy dissipation happens mainly in the $p-$ variable, whereas $\frac{|q|^2}{2}$ is asymptotically conserved.

THE COLLISION OPERATOR

$$Q[f](X,P) = \int S(f,P,P')f(X,P') - S(f,P',P)f(X,P)\,dP'$$

$S(f,P,P') = s(f,P,P')\delta(\frac{|P|^2}{2} - \frac{|P'|^2}{2} \pm \omega)$, ω: amount of energy exchanged with the bath during a collision.

rescale:

$$S(f,P,P') = s\delta(\frac{|p^2|}{2} + \frac{|q^2|}{2\varepsilon} - \frac{|p'|^2}{2} + \frac{|q'|^2}{2\varepsilon} \pm \omega) \approx s\delta(q^2 - {q'}^2)$$

Q conserves asymptotically $\frac{|q|^2}{2}$

$$\int \frac{|q|^2}{2} Q[f](x,y,p,q)\,dpq = O(\varepsilon)$$

STRONG CONFINEMENT

Strong confinement potential

$\Rightarrow$ Forces acting on the particle in the confinement direction y much larger than in the transport direction x.

$$\boxed{V(x,y) = V_0(x) + \frac{1}{\varepsilon} V_1(x,y), \quad \int V_1(x,y)\,dy = 0,\ \forall x}$$

$V_0(x)$: average potential ($V(x,y)$ averaged in y for each x).

$$\boxed{\mathcal{E} \longrightarrow \mathcal{E}_x + \frac{1}{\varepsilon}\mathcal{E}_y}$$

$$\mathcal{E}_x(x,p) = V_0(x) + \frac{|p|^2}{2}, \quad \mathcal{E}_y(x,y,q) = V_1(x,y) + \frac{|q|^2}{2}$$

Scaled Model Equations$_{17}$

$$\boxed{\partial_t f + \{\mathcal{E}_x, f\}_{xp} = \frac{1}{\varepsilon}\mathcal{C}[f] = \frac{1}{\varepsilon}(\{\mathcal{E}_y, f\}_{yq} + Q[f])}$$

$$\mathcal{E}_x(x,p) = V_0(x) + \frac{|p|^2}{2}, \quad \mathcal{E}_y(x,y,q) = V_1(x,y) + \frac{|q|^2}{2}$$

Conserved observables:

$$\int \psi(\mathcal{E}_y(x,y,q))\{\mathcal{E}_y, f\}_{yq}\, dyq = 0, \quad \int \psi(|q|^2)Q[f]\, dq = 0$$

$$\boxed{\Rightarrow \int \psi(\mathcal{E}_y(x,y,q))\mathcal{C}[f]\, dyq = 0, \ \forall x \forall \psi}$$

Large time behavior described by density function $n(x, \mathcal{E}_y(x,y,t), t)$ with $\mathcal{E}_y$ as a free variable.

Chapman - Enskog Asymptotics$_{18}$

Principles: $\boxed{\partial_t f + \{\mathcal{E}_x, f\}_{xp} = \frac{1}{\varepsilon}\mathcal{C}[f]}$

$\mathcal{P}$: Projection onto the kernel - manifold $\mathcal{K}$ of $\mathcal{C}$. Conserves observables: $\mathcal{P}\mathcal{C} = 0$, $\mathcal{C}\mathcal{P} = 0$

$$f = f_0 + \varepsilon f_1, \quad f_0 = \mathcal{P}[f], \quad \varepsilon f_1 = (id - \mathcal{P})[f]$$

$$\boxed{(1)\ \partial_t f_0 + \varepsilon \mathcal{P}[\{\mathcal{E}_x, f_1\}_{xp}] = 0}$$

$$\boxed{(2)\ \varepsilon \partial_t f_1 + \{\mathcal{E}_x, f_0\}_{xp} + \varepsilon (id - \mathcal{P})[\{\mathcal{E}_x, f_1\}_{xp}] = D\mathcal{C}(f_0)[f_1]}$$

(1) slow dynamics on kernel manifold, (2) fast dynamics on the orthogonal complement.

Large time dynamics: The kernel$_{20}$

$$\boxed{\partial_t f_0 + \mathcal{P}[\{\mathcal{E}_x, f_1\}_{xp}] = 0, \quad f_1 = D\mathcal{C}[f_0]^+\{\mathcal{E}_x, f_0\}_{xp}}$$

Projection:

$$\boxed{f_0 = \mathcal{P}[f](x,y,p,q) = \frac{n(x,\mathcal{E}_y(x,y,q),t)}{N(x,\mathcal{E}_y(x,y,q))} M(p)}$$

$n(x,\eta,t)$: density averaged over equi - potential surfaces

$\mathcal{E}_y(x,y,q) = \eta$.

$$\boxed{\int \delta(\mathcal{E}_y - \eta)(id - \mathcal{P})[f]\, dypq = 0, \; \forall x, \eta}$$

N: Density of States (DOS) function, $M(p)$: Maxwellian

$$N(x,\eta) = \int \delta(\mathcal{E}_y(x,y,q) - \eta)\, dyq$$

The Diffusion Equation$_{22}$

$$\partial_t f_0 + \mathcal{P}[\{\mathcal{E}_x, f_1\}_{xp}] = 0, \quad f_1 = DC[f_0]^+\{\mathcal{E}_x, f_0\}_{xp}$$

Diffusion equation for macroscopic density $n(x, \eta, t)$ on large time scales.

$$\boxed{\partial_t n + \nabla_x \cdot F_x + \partial_\eta F_\eta = 0}$$

$$\boxed{F_x = F_x(\nabla_x n, \partial_\eta n), \quad F_\eta = F_\eta(\nabla_x n, \partial_\eta n)\ .}$$

- General formalism.
- Practical problem: Computation of the pseudo - inverse $DC[f_0]^+$

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Computational Complexity$_{23}$

Fluxes have to be computed from

$$\boxed{(id - \mathcal{P})\{\mathcal{E}_x, f_0\}_{xp} = D\mathcal{C}[f_0]f_1, \quad D\mathcal{C}[f_0]f_1 = \{\mathcal{E}_y, f_1\}_{yq} + DQ[f_0]f_1}$$

- No exact solution.
- Represents a $2 \cdot dim(y) - 1$ dimensional problem. Has to be solved for any gridpoint in (x, η)!
- Feasible for thin films ($dim(y) = 1$) but not for channels ($dim(y) = 2$).

Harmonic confinement potentials$_{25}$

Replace $V_1(x, y, q)$ by a quadratic

$$\boxed{V_1(x, y) \rightarrow \frac{1}{2}(y - b(x))^T G(x)(y - b(x))}$$

Choice of b and G:

For every gridpoint in the transport direction x, solve an L^2 minimization problem for the forces in the confinement direction y.

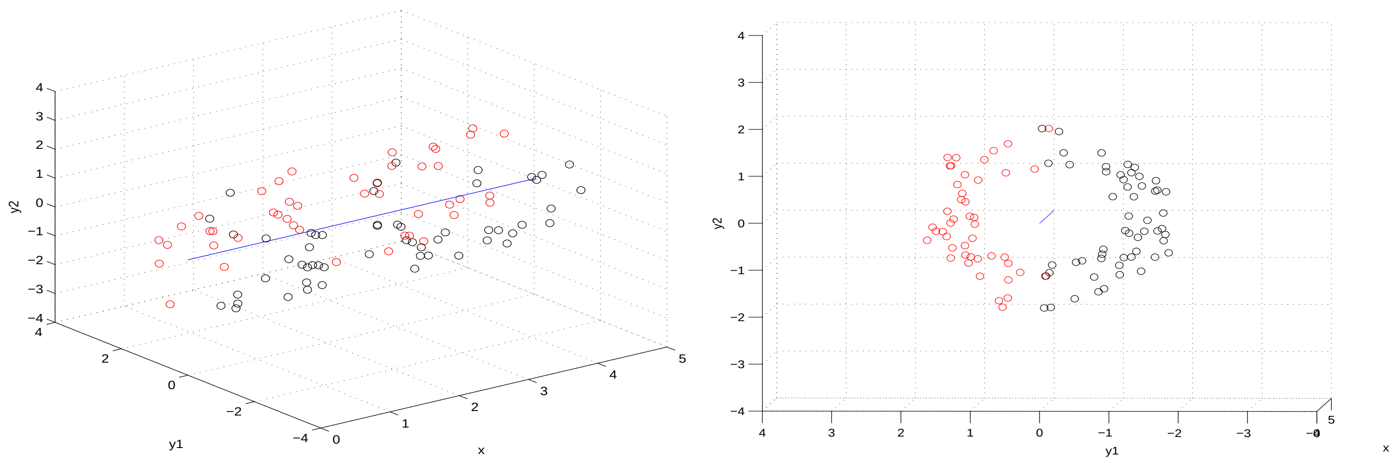
$$\boxed{\int_{\Omega_y} |\nabla_y V_1(x, y) - G(x)(y - b(x))|^2 \, dy \rightarrow \min, \ \forall x}$$

$$\boxed{V_1(x,y) \rightarrow \frac{1}{2}(y-b(x))^T G(x)(y-b(x))}$$

- Equipotential surfaces become ellipsoids in $\mathbb{R}^4$.
- The function f_1 can be parameterized with 3 dimensional angle in $\mathbb{R}^4$.
- Inversion of $D\mathcal{C}$ reduces to a 1-D problem in the azimuth angle.
- Flux computation reduced to an effective 1-D problem $\longrightarrow$ Galerkin - Legendre in the azimuth angle.

Approximation Quality$_{28}$

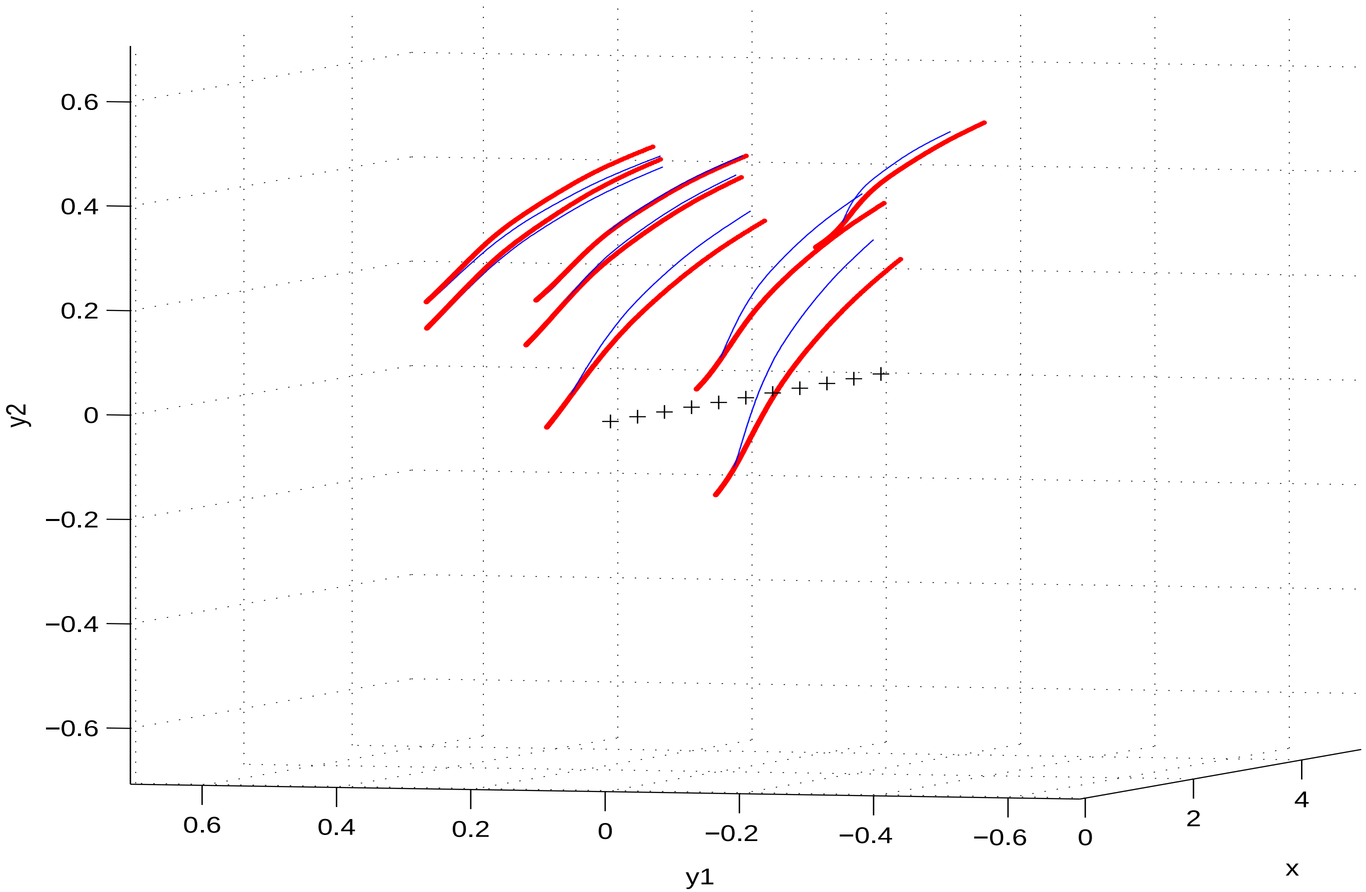
A toy channel



- Generate random charges.
- Compute the exact Coulomb Potential $V(x, y)$ corresponding to these charges, and the local quadratic approximation.

Trajectories

Molecular dynamics trajectories ($x' = p,\ p' = -\nabla_x V$) for the exact and approximate Coulomb potential and random initial conditions.



Inversion of the collision operator $DC[f_1]$ 31

$$\mathcal{C}[f_1] = \{\mathcal{E}_y, f_1\}_{yq} + Q[f_1] = \{\mathcal{E}_x, f_0\}_{xp}$$

Variable transformation:

$$(y, q) = \Omega(x, \eta, \theta_1, \theta_2, \theta_3) \text{ mit } \mathcal{E}_y(x, \Omega(x, \eta, \theta)) = \eta$$

- $\mathcal{C}$ diagonal in θ_2, θ_3.
- Inversion of $\mathcal{C}$: Legendre - Galerkin in θ_1.

The large time diffusion system$_{32}$

$$\boxed{\partial_t n + \nabla_x \cdot F_x + \partial_\eta F_\eta = 0}$$

$$F_x = -N D_x \nabla_x \frac{n}{N} - N \mu_x (1 + \partial_\eta) \frac{n}{N},$$

$$F_\eta = -N D_\eta (1 + \partial_\eta) \frac{n}{N} - N \mu_\eta \cdot \nabla_x \frac{n}{N},$$

- $N, D_x, D_\eta, \mu_x, \mu_\eta$ Functionals of $G(x), b(x)$ (and of V, computed numerically).
- Yields a parabolic system for n.

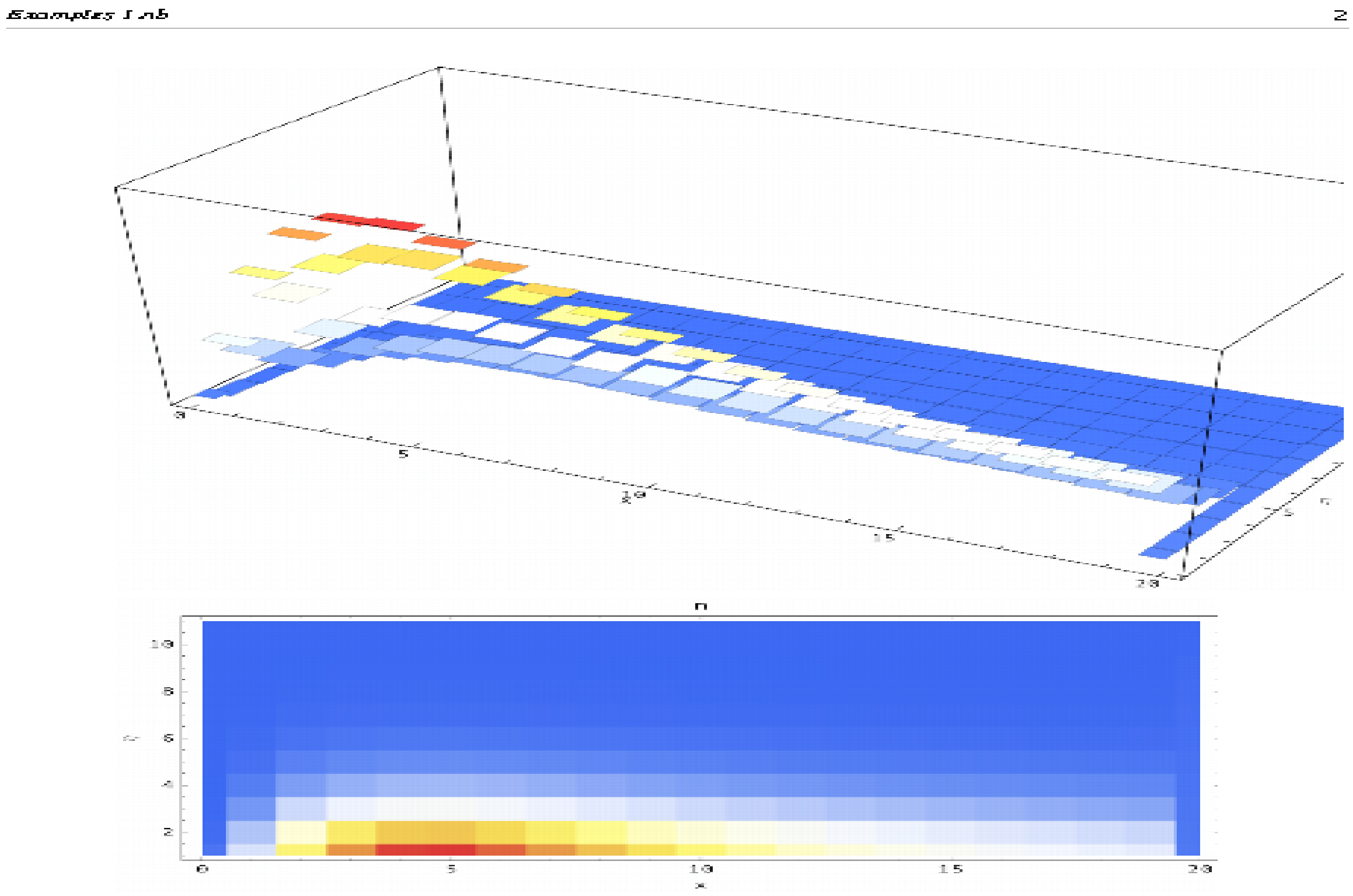
Entropy and Parabolicity$_{33}$

Theorem:(CR, SIAP09)

$$\boxed{\partial_t \int \frac{e^{V_0} n(x,\eta)^2}{N(x,\eta)}\, dx\eta \le 0}$$

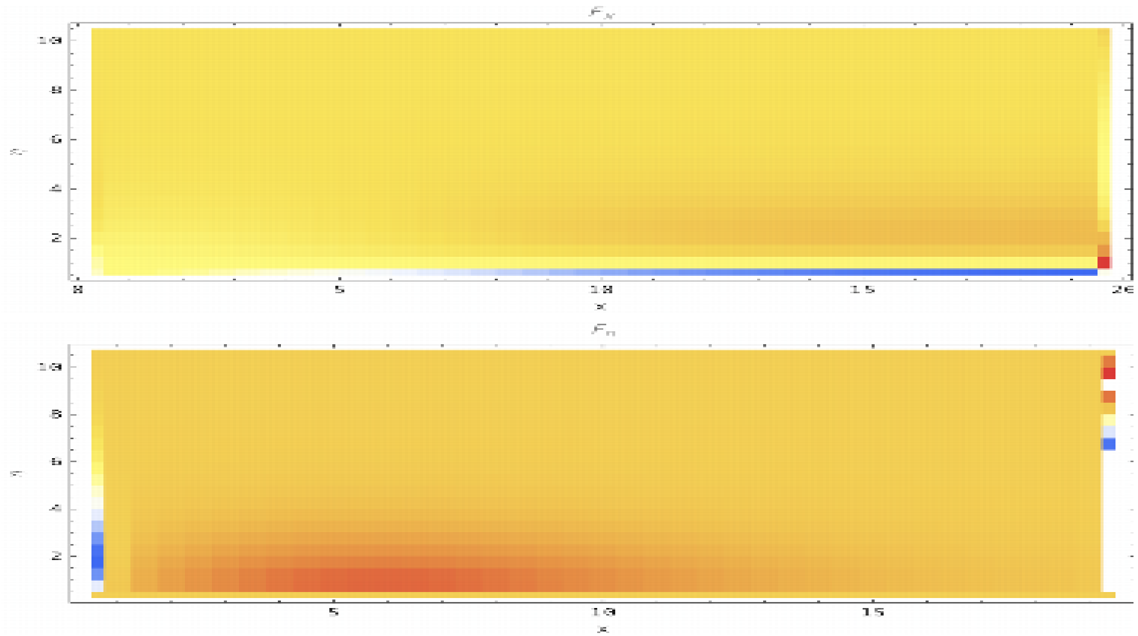
- (implies) $\begin{pmatrix} D_x & \mu_x \\ D_\eta & \mu_\eta \end{pmatrix} \ge 0$

Numerical Results (Density n)$_{33}$



Numerical Results (Fluxes F_x, F_η)

Examples I.nb 6



```
Source current Js: -293.635

Drain current Jd:  -293.635

Jd-Js: 4.17731×10^-9

In[45]:= subbandWire[Lx → 20, Lη → 10, dx → 0.25, dη → 0.25]
Options: {dx → 1, dη → 1, Lx → 5, Lη → 5, silent → False, verbose → True, plotOptions → {}}
Arguments: {Lx → 20, Lη → 10, dx → 0.25, dη → 0.25}
Nx: 81
Nη: 41
```

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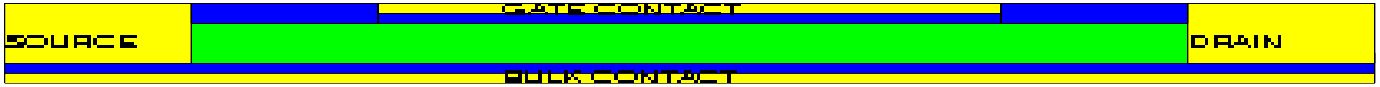
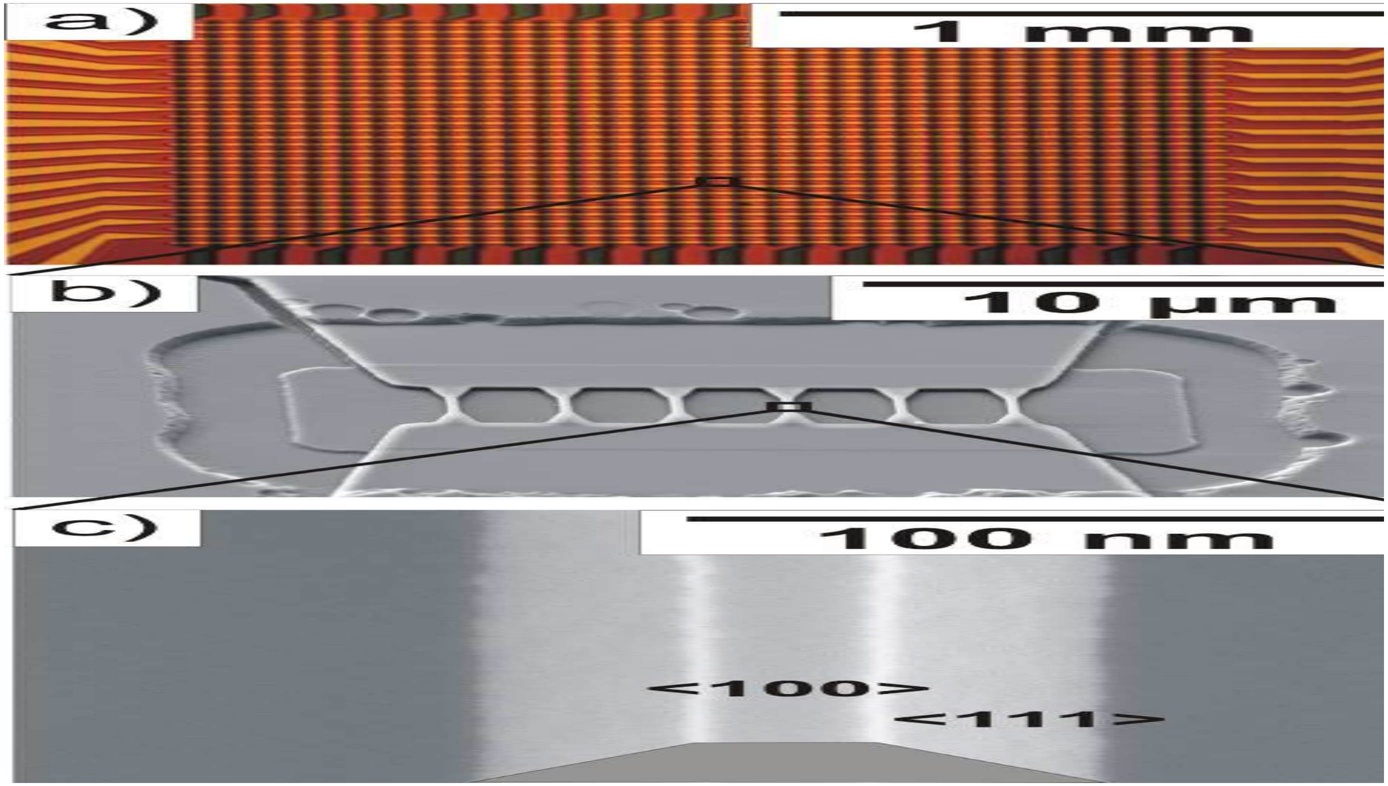
Part 3: Thin Films$_{36}$



1

Nanowire Arrays



1

A slightly different problem$_{35}$

- Goal: large time asymptotics for conserved quantities (energy tensor in confinement direction).
- V_1: Step function potential, jump in the bandgap energy from semiconductor to oxide.
- Much much smaller length scales. Classical transport description insufficient $\longrightarrow$ q.m. transport picture.
- Q.m. collision mechanisms very complicated.

The quantum transport picture $_{37}$

The Schrödinger equation:

$$\boxed{i\hbar\partial_t\rho = \{\mathcal{H}_x, \rho\} + \frac{1}{\varepsilon}\mathcal{C}[\rho], \quad \mathcal{C}[\rho] = \{\mathcal{H}_y, \rho\} + Q[\rho]}$$

$$\mathcal{H}_x = -\frac{{h_x}^2}{2m}\Delta_x + V_0(x), \quad \mathcal{H}_y = -\frac{{h_y}^2}{2m}\Delta_y + \frac{1}{\varepsilon}V_1(x,y),$$

$\rho(x, y, x', y')$ density matrix for the mixed state.

h_x, h_y scaled Planck constants (relative to the length and energy scales in x and y).

$$h_x = O(\varepsilon), \quad h_y = O(1)$$

$h_x \rightarrow 0 \rightarrow$ classical diffusion system in x while retaining the q.m. transport in y.

Sub-band modeling

.

$$\boxed{\partial_t n_k + \nabla_x \cdot F_k = 0, \quad F_k = -\nabla_x n_k - n_k E_k}$$

$$H_y \psi_k(x,y) = E_k(x) \psi_k(x,y)$$

- (Fischetti Phys. Rev. B, (1999),
- BenAbdallah, Mehats, Schmeiser, Vauchelet,Weisshäupl, SIAP (2005)).
- Additional effects: large confinement forces, thermodynamics.

Conserved Observables$_{39}$

- Analogy to classical case: $\mathcal{H}_y$ (energy in the confinement direction).
- Components of the wave function in the eigenspaces of $\mathcal{H}_y$.

$\psi_k(x,y)$: eigenfunction and $E_k(x)$: eigenvalue

$$\mathcal{H}_y \psi_k(x,y) = E_k(x)\psi_k(x,y)$$

$$\boxed{\int \psi_k(x,y)\mathcal{C}[\rho](x,y,x,y')\psi_k(x,y')\, dyy' = 0,\ \forall x, k}$$

$$\Longleftrightarrow\ Tr(\Phi(x,\mathcal{H}_y)\mathcal{C}[\rho]) = 0, \quad \forall x,\ \forall \Phi : \mathbb{R}^2 \to \mathbb{R}$$

classical: $\int \phi(x,p,\mathcal{E}_y)\mathcal{C}[f]\, dxypq = 0, \forall \phi$

The Collision Operator$_{40}$

Q.M. collisions hard to secribe on the level of the Schrödinger or Heisenberg equation. (NEGF, Lindblad...)

Relaxation - operator

$$\boxed{\mathcal{C}[\rho] = \frac{1}{\tau}(\mathcal{M}[\rho] - \rho)}$$

$\mathcal{M}[\rho]$: Local thermodynamic equilibrium. Maximizes the relative Von Neumann entropy under the constraint of given observables.

$$Tr[\mathcal{M}\cdot(id+\mathcal{H}-\ln(\mathcal{M}))] \to \max,\ \forall \mathcal{M} : Tr[\phi(\mathcal{H}_y)(\mathcal{M}-\rho)] = 0,\ \forall \phi$$

(QM - generalization of the Levermore closures)

Theorem :

$$Tr[\mathcal{M}\cdot(id+\mathcal{H}-\ln(\mathcal{M}))] \rightarrow \max,\ \forall\mathcal{M} : Tr[\phi(\mathcal{H}_y)(\mathcal{M}-\rho)] = 0,\ \forall\phi$$

Degond, CR (JMP03):

The optimization problem has a unique solution, given in terms of

chemical potential operators.

$$\boxed{\mathcal{M}[\rho] = \exp[-\mathcal{H}_x + \phi_\rho(\mathcal{H}_y)], \quad \phi_\rho : Tr_y(\mathcal{M}[\rho]) = Tr_y(\rho)}$$

Confined Quantum - Energy Transport$_{42}$

$$i\varepsilon\partial_t\rho = \{\mathcal{H}_x, \rho\} + \frac{1}{\varepsilon}\mathcal{C}[\rho], \quad \mathcal{C}[\rho] = -\{\mathcal{H}_y, \rho\} + \frac{i}{\tau}(\mathcal{M}[\rho] - \rho)$$

- Instead of $n(x,\eta)$ in the classical case, asymptotics yields a system for $n_k, \; k \in \mathbb{N}$, the components of the density belonging to eigenspace k.

$$n_k(x) = \int \psi_k(x,y)\rho(x,y,x,y')\psi_k(x,y')\, dyy' = 0, \; \forall x, k$$

$$\partial_t n_k + \nabla_x \cdot (F_k^x[n]) + F_k^\eta[n] = 0$$

The Semiclassical Limit $h_x \to 0,\ h_y = O(1)$

The classical limit in the transport direction, leaving transport in the confinement direction fully q.m., gives the fluxes F_k^x and F_k^η.

$$\boxed{\partial_t n_k + \nabla_x \cdot F_k^x[n] + F_k^\eta[n] = 0,\ F_k^x[n] = -\nabla_x n_k - n_k \nabla_x E_k}$$

$$\boxed{F_k^\eta[n] = -\sum_j |A_{kj}|^2 (n_j - n_k)(1 + \frac{E_j - E_k}{\ln(n_j) - \ln(n_k)})}$$

- $F_k^\eta = 0 \Rightarrow$: standard sub-band equations.
- $F_k^\eta[n]$ models energy transfer between eigenspaces due to large forces in the confinement direction y.

  $\rightarrow$inter - band collision operator, (A_{kj} dependent on eigenfunctions of $\mathcal{H}_y$)

Structure of the Inter - Band Collision Operator$_{44}$

$$\boxed{F_k^\eta[n] = -\sum_j |A_{kj}|^2 (n_j - n_k)\left(1 + \frac{E_j - E_k}{\ln(n_j) - \ln(n_k)}\right)}$$

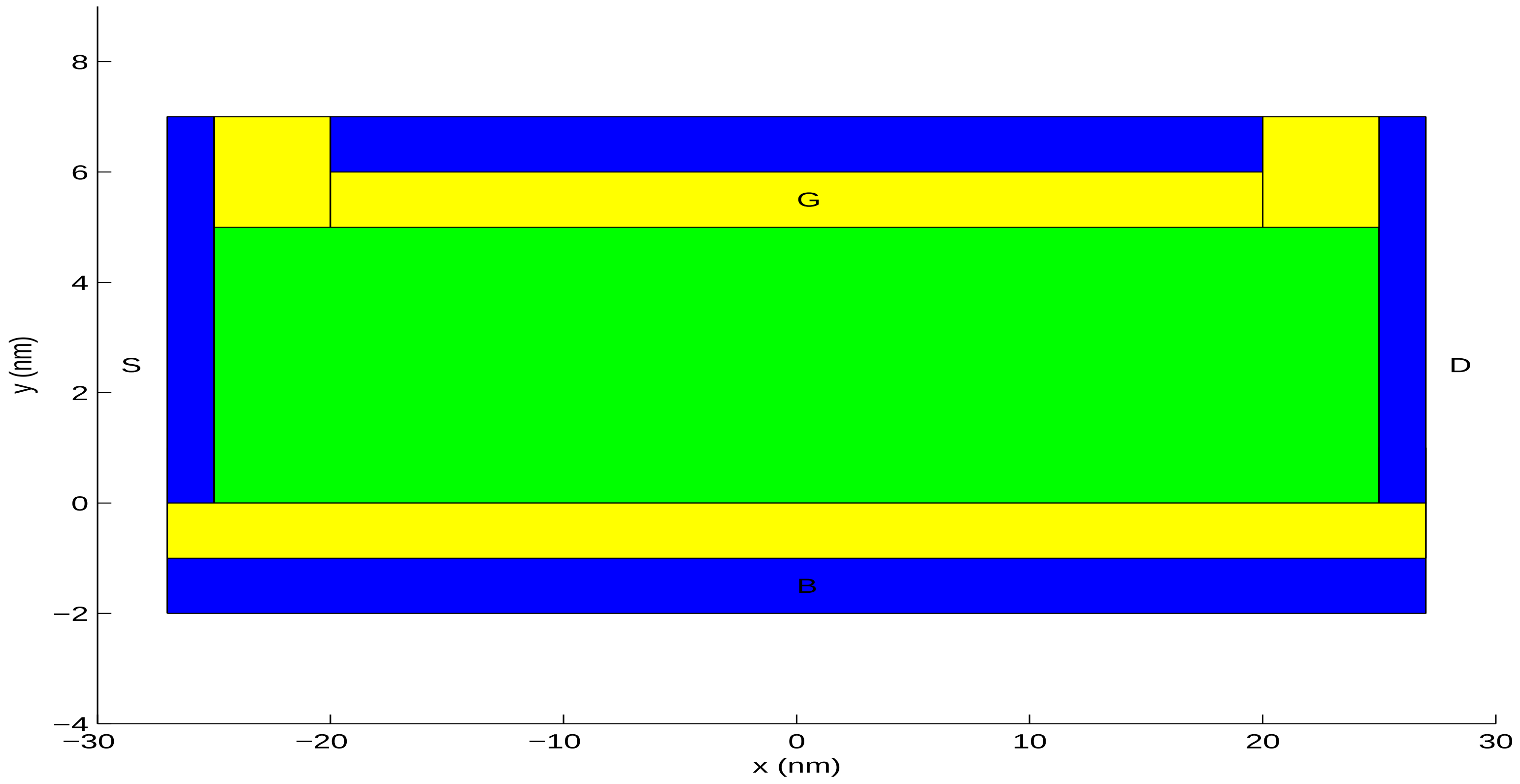
Theorem: (CR, SIAP09)

- Kernel of F^η consists of elements of the form $n_k(x) = c(x)e^{-E_k(x)}$.
- F^η dissipates the entropy functional $G[n] = \sum_k n_k(\ln(n_k) + E_k - 1)$ locally in x.

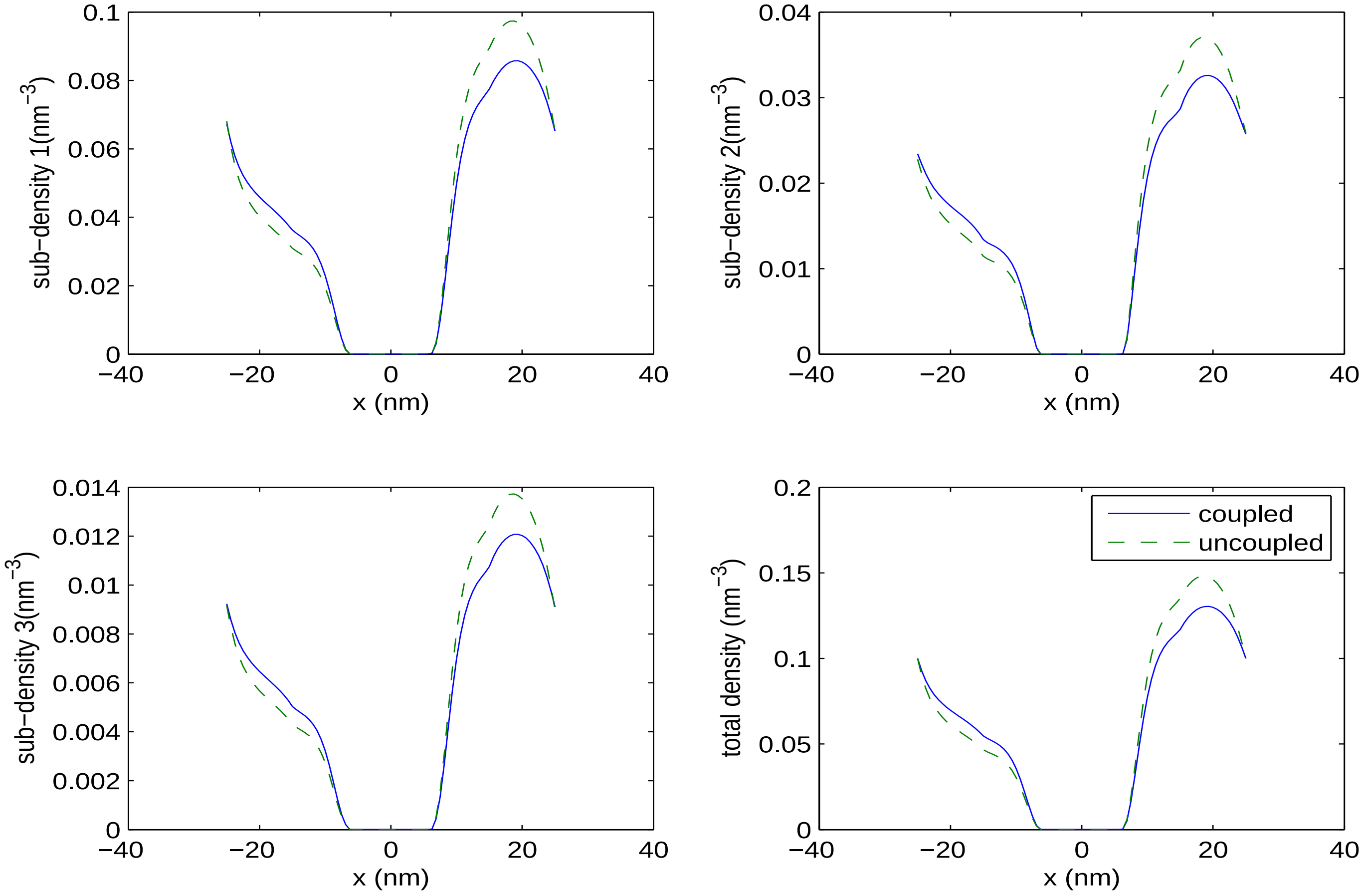
$$\boxed{\sum_k (\ln(n_k) + E_k) F_k^\eta[n] \geq 0, \ \forall x}$$

- $\Rightarrow F^\eta$ relaxes the system against a local Maxwell - Boltzmann distribution $n_k(x) = c(x)e^{-E_k}$.

Example: Thin SOI - Devices

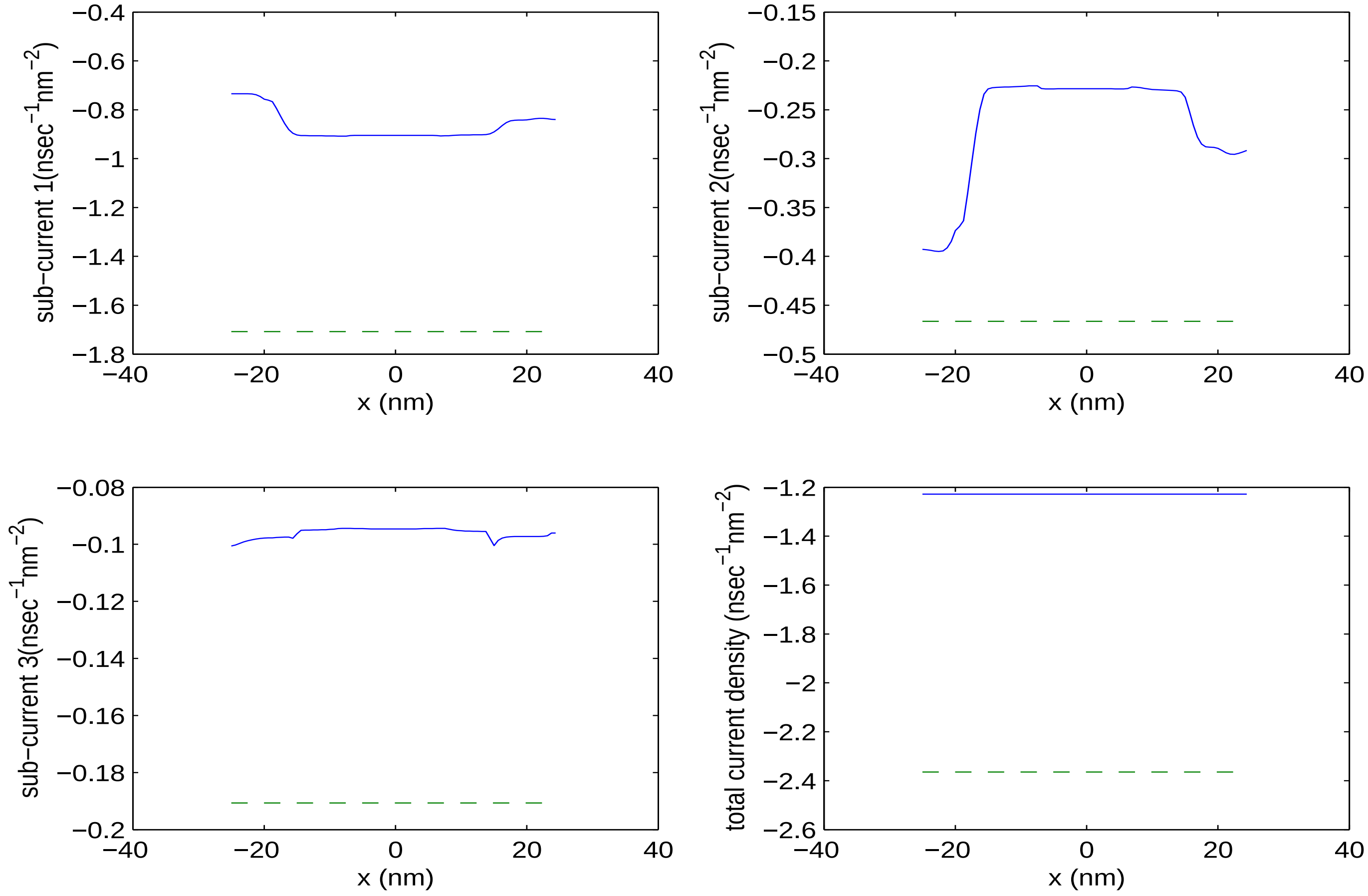


Sub - band densities using 3 sub - bands



Comparison of strong confinement to uncoupled case

Comparison of flux densities.



Conclusions

- General principle of anisotropic energy dissipation yields large time averaged models with energy as additional free variable.
- Incorporates relatively complex micro - geometries into macro models.
- Q1: Improvement over locally parabolic confinement potentials.
- Q2: Does q.m. transport picture add something to the behavior of channels?

Center for Scientific Computation And Mathematical Modeling

Kinetic Description of Multiscale Phenomena: Modeling, Theory, and Computation

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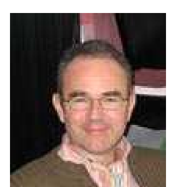
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