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.
Thin tubes: Proteins and Ion channels

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

Protein 1LNQ
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

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

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

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

Classical picture: Newton equations

\[
\begin{align*}
\frac{dX}{dt} &= P, \\
\frac{dP}{dt} &= -\nabla_X \mathcal{E}
\end{align*}
\]

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

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

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

*Q*: Dissipative collision operator (scattering with the background)

**Boltzmann**: Integral operator

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

**Fokker-Planck** (Wiener process, random walk)

\[ Q[f](X, P) = \nabla_P \cdot [\nabla_P f + \gamma P f] \]

*Q* relaxes against some notion of thermodynamic equilibrium \( \Rightarrow \) large time asymptotics.
OUTLINE

- Part 1: General principles
  - Confined geometries, anisotropic energy dissipation → fluid models with free energy variables.

- Part 2: Classical transport in narrow channels.

  - Conservation laws and local entropies.
CONFINED GEOMETRIES

\[ X = (x, y) \in \Omega = \Omega_x \times \Omega_y \text{ with } |\Omega_y| \ll |\Omega_x| \]

\( x \): transport direction, \( y \): confinement direction.

\[ P = (p, q) \]

- Thin films: \( x, p \in \mathbb{R}^2, y, q \in \mathbb{R}^1 \)
- Narrow channels: \( x, p \in \mathbb{R}^1, y, q \in \mathbb{R}^2 \)
\( y \ll x \rightarrow y = O(\varepsilon) \)

\( \varepsilon \): aspect ratio

Rescale:

\[
\begin{align*}
    y & \rightarrow \frac{y}{\varepsilon}, \\
    q & \rightarrow \frac{q}{\sqrt{\varepsilon}}, \\
    t & \rightarrow \frac{t}{\varepsilon}
\end{align*}
\]

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

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

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

rescale:

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

\( Q \) 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

⇒ Forces acting on the particle in the confinement direction \( y \) much larger than in the transport direction \( x \).

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

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

\[
\mathcal{E} \rightarrow \mathcal{E}_x + \frac{1}{\varepsilon} \mathcal{E}_y
\]

\[
\mathcal{E}_x(x, p) = V_0(x) + \frac{|p|^2}{2}, \quad \mathcal{E}_y(x, y, q) = V_1(x, y) + \frac{|q|^2}{2}
\]
Scaled Model Equations

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

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

Conserved observables:

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

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

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

\[ \partial_t f + \{ \mathcal{E}_x, f \}_x p = \frac{1}{\varepsilon} \mathcal{C}[f] \]

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

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

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

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

\[ (2) \varepsilon \partial_t f_1 + \{ \mathcal{E}_x, f_0 \}_x p + \varepsilon (id - \mathcal{P})[\{ \mathcal{E}_x, f_1 \}_x p] = D \mathcal{C}(f_0)[f_1] \]
Large time dynamics: The kernel

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

Projection:

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

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

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

\[
\int \delta(\mathcal{E}_y - \eta)(id - \mathcal{P})[f] \, dp dq = 0, \quad \forall x, \eta
\]

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

\[
N(x, \eta) = \int \delta(\mathcal{E}_y(x, y, q) - \eta) \, dy q
\]
The Diffusion Equation

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

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

\[ \partial_t n + \nabla_x \cdot F_x + \partial_\eta F_\eta = 0 \]

\[ F_x = F_x(\nabla_x n, \partial_\eta n), \quad F_\eta = F_\eta(\nabla_x n, \partial_\eta n). \]

- General formalism.
- Practical problem: Computation of the pseudo-inverse \( DC[f_0]^+ \)
Part 1: General principles

- Confined geometries, anisotropic energy dissipation → fluid models with free energy variables.

Part 2: Classical transport in narrow channels.


- Conservation laws and local entropies.
Fluxes have to be computed from

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

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

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

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

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 $y$.

$$\int_{\Omega_y} |\nabla_y V_1(x, y) - G(x)(y - b(x))|^2 dy \rightarrow \min, \ \forall x$$
\[ V_1(x, y) \rightarrow \frac{1}{2} (y - b(x))^T G(x) (y - b(x)) \]

- 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 \( DC \) reduces to a 1-D problem in the azimuth angle.
- Flux computation reduced to an effective 1-D problem \( \rightarrow \) Galerkin - Legendre in the azimuth angle.
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 $DC[f_1]_{31}$

$$C[f_1] = \{E_y, f_1\}_{yq} + Q[f_1] = \{E_x, f_0\}_{xp}$$

Variable transformation:

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

- $C$ diagonal in $\theta_2, \theta_3$.
- Inversion of $C$: Legendre - Galerkin in $\theta_1$. 
The large time diffusion system

\[ \partial_t n + \nabla_x \cdot F_x + \partial_\eta F_\eta = 0 \]

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

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

- \( N, D_x, D_\eta, \mu_x, \mu_\eta \) Functionals of \( G(x), b(x) \) (and of \( V \), computed numerically).

- Yields a parabolic system for \( n \).
Entropy and Parabolicity

Theorem: (CR, SIAP09)

\[ \partial_t \int e^{V_0 n(x,\eta)} \frac{n(x,\eta)^2}{N(x,\eta)} \, dx \eta \leq 0 \]

\( \implies \) (implies)

\[ \begin{pmatrix} D_x & \mu_x \\ D_\eta & \mu_\eta \end{pmatrix} \geq 0 \]
Numerical Results (Density $n_{33}$)
Numerical Results (Fluxes $F_x, F_\eta$)

```
Source current js: -292.105
Drain current Id: -287.675
Jo-Js: -4.43733e-09

mp45m: subbandWire(Lx = 20, Ld = 10, dx = 0.25, dy = 0.25)
Options: dj = 1, dj = 1, Lx = 2, Ld = 2, silent = false, verbose = true, plot2Dplot = $\{1\}$
Arguments: Lx = 20, Ld = 10, dx = 0.25, dy = 0.25
max = 41
n1 = 41
```
Part 1: General principles

• Confined geometries, anisotropic energy dissipation → fluid models with free energy variables.

Part 2: Classical transport in narrow channels.

• Computational complexity. Locally harmonic potential approximation. Numerics.


• Conservation laws and local entropies.
Part 3: Thin Films

[Diagram of a transistor structure showing layers for source, gate, channel, drain, and contact areas.]

1
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 $\rightarrow$ q.m. transport picture.

Q.m. collision mechanisms very complicated.
The Schrödinger equation:

\[
\begin{align*}
\dot{\rho} &= \left\{\mathcal{H}_x, \rho\right\} + \frac{1}{\varepsilon} C[\rho], \\
C[\rho] &= \left\{\mathcal{H}_y, \rho\right\} + Q[\rho]
\end{align*}
\]

\[
\begin{align*}
\mathcal{H}_x &= -\frac{\hbar_x^2}{2m} \Delta_x + V_0(x), \\
\mathcal{H}_y &= -\frac{\hbar_y^2}{2m} \Delta_y + \frac{1}{\varepsilon} V_1(x, y),
\end{align*}
\]

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

\(\hbar_x, \hbar_y\) scaled Planck constants (relative to the length and energy scales in \(x\) and \(y\)).

\[
\begin{align*}
\hbar_x &= O(\varepsilon), \\
\hbar_y &= O(1)
\end{align*}
\]

\(\hbar_x \to 0 \to\) classical diffusion system in \(x\) while retaining the q.m. transport in \(y\).
Sub-band modeling

\[ \partial_t n_k + \nabla_x \cdot F_k = 0, \quad F_k = -\nabla_x n_k - n_k E_k \]

\[ H_y \psi_k(x, y) = E_k(x) \psi_k(x, y) \]

► (Fischetti Phys. Rev. B, (1999),

► BenAbdallah, Mehats, Schmeiser, Vauchelet, Weisshäupl, SIAP (2005)).

► Additional effects: large confinement forces, thermodynamics.
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

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

$$\int \psi_k(x, y) C[\rho](x, y, x, y') \psi_k(x, y') dy y' = 0, \forall x, k$$

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

classical: $$\int \phi(x, p, \mathcal{E}_y) C[f] dxy pq = 0, \forall \phi$$
The Collision Operator

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

Relaxation - operator

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

\( M[\rho] \): Local thermodynamic equilibrium. Maximizes the relative Von Neumann entropy under the constraint of given observables.

\[ Tr[M \cdot (id + H - \ln(M))] \rightarrow \max, \ \forall M : Tr[\phi(H_y)(M - \rho)] = 0, \ \forall \phi \]

(QM - generalization of the Levermore closures)
Theorem:

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

Degond, CR (JMP03):

The optimization problem has a unique solution, given in terms of chemical potential operators.

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

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

\[ n_k(x) = \int \psi_k(x, y) \rho(x, y, x, y') \psi_k(x, y') \, dyy' = 0, \quad \forall x, k \]

\[ \partial_t n_k + \nabla_x \cdot (F^x_k[n]) + F^\eta_k[n] = 0 \]
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 $F^{x}_k$ and $F^{\eta}_k$.

\[
\partial_t n_k + \nabla_x \cdot F^{x}_k[n] + F^{\eta}_k[n] = 0, \quad F^{x}_k[n] = -\nabla_x n_k - n_k \nabla_x E_k \\
F^{\eta}_k[n] = -\sum_j |A_{kj}|^2 (n_j - n_k) \left(1 + \frac{E_j - E_k}{\ln(n_j) - \ln(n_k)}\right)
\]

$F^{\eta}_k = 0 \implies$ standard sub-band equations.

$F^{\eta}_k[n]$ models energy transfer between eigenspaces due to large forces in the confinement direction $y$.

$\to$ inter-band collision operator, ($A_{kj}$ dependent on eigenfunctions of $\mathcal{H}_y$)
Structure of the Inter-Band Collision Operator

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

**Theorem:** (CR, SIAP09)

- Kernel of \( F^\eta \) consists of elements of the form
  \[ n_k(x) = c(x)e^{-E_k(x)} \].

- \( F^\eta \) dissipates the entropy functional
  \[ G[n] = \sum_k n_k(\ln(n_k) + E_k - 1) \text{ locally in } x. \]
  \[ \sum_k (\ln(n_k) + E_k) F^\eta_k[n] \geq 0, \forall x \]

- \( F^\eta \) 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?
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