LECTURE III
ENTROPY AND MOMENT CLOSURES

QUANTUM MECHANICS FOR MIXED STATES

The Schrödinger equation:

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta_x\psi + \phi(x)\psi$$

Mixed states and density matrices:

$$\rho(x,y,t) = \sum_n \psi_n(x,t)\gamma_n\psi_n^*(y,t)$$

γ_n: occupation probability of the state n.

The Heisenberg equation:

$$i\hbar\partial_t\rho = \{H,\rho\} = H\cdot\rho - \rho\cdot H, \quad H\cdot\rho(x,y,t) = \int H(x,z)\rho(z,y,t)\,dz$$

OUTLINE

- Macroscopic approximations. Moment closures and asymptotics using BGK operators,based on entropy principles.

- Relate moments (classical) to a quantum mechanical entropy.

- The Wigner - Weyl formalism. Algebraic properties. Weyl calculus.

- Applications: Extended quantum hydrodynamics and effective potentials

WIGNER TRANSFORM AND WEYL QUANTIZATION

The Wigner transform:

Given any linear operator a with an integral kernel (a density matrix) $a_d(x,y)$, i.e. $a(\psi)(x) = \int a_d(x,y)\psi(y)\ dy$, we define the corresponding Wigner function

$$W[a](x,\xi) = \int a(x-\frac{1}{2}y, x+\frac{1}{2}y)e^{iy\cdot\xi}\,dy, \quad f(x,\xi,t) = W[\rho](x,\xi,t)$$

Conversely, given any function $g(x,\xi)$ we define the corresponding density matrix and operator via the inverse Wigner transform

$$W^{-1}[g](r,s) = (2\pi)^{-d}\int g(\frac{r+s}{2},\xi)e^{i\xi\cdot(r-s)}\ d\xi$$

Advantages

- Relates quantum mechanical transport picture to classical picture.

- Allows directly (at least on a formal level) for the classical limit $\hbar \longrightarrow 0$.

- Linear algebra.

Rules

1. Self adjoint operators and density matrices correspond to real functions.

$$a(r,s) = a(s,r)^* \iff W[a](x,\xi) \in \mathbb{R}$$

2. Matrix products (operator composition) transform into Wigner - Weyl products.

$$c = a \cdot b, \quad c(x,y) = \int a(x,z)b(z,y)\ dz$$

$$W[c] = W[a] \circ W[b] = a(x+\frac{i}{2}\nabla_\xi, \xi-\frac{i}{2}\nabla_x)b(x,\xi)$$

$$= b(x-\frac{i}{2}\nabla_\xi, \xi+\frac{i}{2}\nabla_x)a(x,\xi)$$

Pseudo differential operator notation:

$$W[a] \circ W[b] =$$

$$(2\pi)^{-2d} \int a(x-\frac{1}{2}r, \xi+\frac{1}{2}\eta)b(x',\xi') \exp[r\cdot(\xi-\xi')+\eta\cdot(x-x')]\ dx'\eta d\xi' r$$

3. Traces of matrix products become L^2 products

$$Tr(a \cdot b) = \int a_d(r,s)b_d(s,r)\ drs = (2\pi)^{-3} \int W[a](x,\xi)W[b](x,\xi)\ dx\xi$$

4. The Wigner commutator

$$a(x,\xi) = W[a_d], \quad b(x,\xi) = W[b_d], \quad \{a,b\}_W = W[\{a_d, b_d\}]$$

$$\{a,b\}_W = \sum_{\sigma=\pm 1} \sigma a(x + \frac{i\sigma}{2}\nabla_\xi, \xi - \frac{i\sigma}{2}\nabla_x) b(x,\xi)$$

Example:

$$H(x,y) = -\frac{\hbar^2}{2m}\Delta\delta(x-y) + \phi(x)\delta(x-y), \quad W[H] = \frac{\hbar^2|\xi|^2}{2m} + \phi(x)$$

$$i\hbar\partial_t f = [-\frac{\hbar^2}{m} i\xi \cdot \nabla_x + \sum_{\sigma=-1}^{1} \sigma\phi(x + \frac{i\sigma}{2}\nabla_\xi)]f$$

$\hbar\xi = mv = p,\ \nabla_\xi = \hbar\nabla_p$

$$\partial_t f = [-\frac{p}{m} \cdot \nabla_x + \frac{1}{i\hbar} \sum_{\sigma=\pm 1} \sigma\phi(x + \frac{i\hbar\sigma}{2}\nabla_p)]f$$

MOMENT CLOSURES

$$\partial_t f + \{H, f\}_{(W)} = Q[f]$$

$Q[f]$: Dissipative operator, models particle interactions.

Macroscopic Approximations: Derive equations for functionals (moments) of the kinetic density function f. Yields to lower dimensional equations which are computationally more feasible.

$$\partial_t m_j + L_j(\mathbf{m}) = Q_j(\mathbf{m}), \quad j = 0, .., J$$

$\mathbf{m} = (m_0, .., m_J)$: Functionals of f; usually local moments; $m_j(x,t) = \int \kappa_j(p) f(x,p,t)\ dp$
L_j, Q_j : Corresponding functionals of L, Q,
i.e. $L_j(x,t) = \int \kappa_j(p) L[f](x,p,t)\ dp$

The closure problem: How to express L_j, Q_j in terms of the moments $\mathbf{m}$.

THE CLASSICAL APPROACH

The (dissipative) collision operator Q drives the solution towards the kernel manifold $\mathcal{M}$ of Q.

Close the moment hierarchy by parameterizing $\mathcal{M}$ in terms of the moments.

$$Q[f] = 0 \iff f(x,\xi,t) = \mathcal{M}(\mathbf{m}(x,t),\xi), \quad \int \kappa \mathcal{M}(\mathbf{m},\xi)\, d\xi = \mathbf{m}$$

$$L_j(\mathbf{m}) = \int \kappa_j \{H, \mathcal{M}(\mathbf{m},\xi)\}\, d\xi, \quad Q_j(\mathbf{m}) = \int \kappa_j Q[\mathcal{M}(\mathbf{m},\xi)]\, d\xi \; (= 0)$$

The classical case:

$\mathcal{M}$ (the local Maxwellian), parameterized by mass, momentum and energy. $f(x,\xi,t) = \frac{n}{\sqrt{2\pi T}} \exp[-\frac{|v-u|^2}{2T}]$, $v = \frac{\hbar\xi}{m}$.

$$\mathbf{m}(n,u,T) = \frac{n}{\sqrt{2\pi T}} \int \begin{pmatrix} 1 \\ \xi \\ \frac{|\xi|^2}{2} \end{pmatrix} \exp[-\frac{|v-u|^2}{2T}] \, d\xi$$

Yields the compressible Euler equations (the hydrodynamic model).

BGK OPERATORS

$$\partial_t f + \{H, f\}_{(W)} = Q[f] = \frac{1}{\varepsilon}[\mathcal{M}(\mathbf{m}_f, \xi) - f]$$

Gives the same moments.

Asymptotics for $\varepsilon \to 0$ (Chapman - Enskog expansion) $\Rightarrow$ Diffusive terms (Navier Stokes, diffusion equations).

Remark: The only information needed about Q on this level is the shape of the local Maxwellian $\mathcal{M}$.

The problem:

- Scattering on a quantum mechanical level is not very well understood.
- Various models. None render themselves to macroscopic asymptotics.

MAXIMUM LIKELIHOOD CLOSURES

Given a dissipation property (an entropy) the kernel of the collision operator has to maximize the entropy, while conserving a certain set of quantities.

The quantum Von Neumann entropy

$$\rho(x,y) = \sum_n \psi_n(x)\gamma_n\psi_n(y)^*$$

$$S[\rho] = \sum_n \gamma_n(1 - \ln\gamma_n) = Tr[\rho(1 - \ln\rho)]$$

THE LOCAL MAXWELLIAN

Given a certain set of conserved observables (moments) $\mathbf{m}$, the local Maxwellian $\mathcal{M}[\mathbf{m}]$ maximizes entropy, given the moments.

Find $\mathcal{M}[\mathbf{m}] = W[\rho_{\mathbf{m}}]$

$Tr[\rho_{\mathbf{m}}(1-\ln \rho_{\mathbf{m}})] \to$ max constraint: $\int \kappa(\xi) W[\rho_{\mathbf{m}}]\, d\xi = \mathbf{m}(x)$

USE:

- Close the moment system with $\mathcal{M}[\mathbf{m}]$.

- Use

$$Q[f] = \frac{1}{\varepsilon}[\mathcal{M}[\mathbf{m}_f] - f], \quad \mathbf{m}_f = \int \kappa f \; d\xi$$

as phenomenological (BGK) collision operator. (computation, Chapman - Enskog, diffusion approximations)

- Effective energies:

$$\{\mathcal{E}, f\}_W = \{\mathcal{E}^{eff}[\mathbf{m}], f\} \text{ for } f = \mathcal{M}[\mathbf{m}]$$

THE CONSTRAINED OPTIMIZATION PROBLEM

$$S[\rho_{\mathbf{m}}] \to \text{max}, \text{ constraint: } \int \kappa(\xi) W[\rho_{\mathbf{m}}] \, d\xi = \mathbf{m}(x)$$

$$S[\rho_{\mathbf{m}}] = Tr[\rho_{\mathbf{m}}(1 - \ln \rho_{\mathbf{m}})]$$

Lagrange multipliers:
Maximize

$$S[\rho_{\mathbf{m}}] + \int \lambda(x)^T \kappa(\xi) W[\rho_{\mathbf{m}}] \, dx\xi - \int \lambda(x)^T \mathbf{m}(x) \, dx$$

Theorem: (Degond, CR, 03)
Given a function $\phi(z) : \mathbb{R} \to \mathbb{R}$. This induces an operator $\Phi(\rho)$ on the space of self adjoint Hilbert - Schmitt operators. In the same way $\phi'(z)$ induces $\Phi'(\rho)$.

$$\boxed{Tr[D\Phi(\rho)(\Delta\rho)] = Tr[\Phi'(\rho) \cdot \Delta\rho]}$$

$$-Tr[\ln \rho_{\mathbf{m}} \cdot \Delta\rho] + \int \lambda(x)^T \kappa(\xi) W[\Delta\rho] \; dx\xi, \;\; \forall \Delta\rho$$

$$\int \kappa(\xi) W[\rho_{\mathbf{m}}] \; d\xi = \mathbf{m}(x), \;\; \forall x$$

$\Rightarrow$

$$\rho_{\mathbf{m}} = \exp(W^{-1}[\lambda(x) \cdot \kappa(\xi)]), \quad \mathcal{M}[\mathbf{m}] = W[\exp(W^{-1}[\lambda(x) \cdot \kappa(\xi)])]$$

$$\lambda(x) = \lambda_{\mathbf{m}}(x) : \; \int \kappa W[\exp(W^{-1}[\lambda_{\mathbf{m}}(x) \cdot \kappa(\xi)])] \; d\xi = \mathbf{m}(x), \;\; \forall x$$

HOW TO COMPUTE THE EXPONENTIAL OF A MATRIX

Compute the matrix exponential involving $\lambda_{\mathbf{m}}$ such that it satisfies the local moment relations. $\Rightarrow \mathcal{M}[\mathbf{m}]$.

The Bloch equation

- To compute $e^{-\lambda z}$: Solve $\partial_\beta u = -\lambda u, \; u(0) = 1, \; z = u(1)$
- To compute $\exp(-a)$: Solve

$$\partial_\beta u = \frac{1}{2}(-a{\cdot}u - u{\cdot}a), \; u(x, y, \beta = 0) = \delta(x - y), \; e^{-a} = u(x, y, \beta = 1)$$

- To compute $W[e^{-a}]$: Solve

$$\partial_\beta g = \frac{1}{2}(-g \circ W[a] - g \circ W[a]), \; g(x, \xi, \beta = 0) = 1, \; W[e^{-a}] = g(x, y, \beta = 1$$

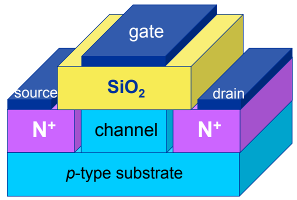
APPLICATIONS

- Use $\mathcal{M}[\mathbf{m}]$ to close moment hierarchy $\Rightarrow$ extended quantum hydrodynamics (equivalent of the Levermore closures in the q.m. case). (Degond, CR, Jüngel, Milisic).

- Use $\mathcal{M}[\mathbf{m}]$ in a BGK operator, Chapman - Enskog expansion $\Rightarrow$ quantum diffusion equations (Gallego, Mehats).

- Use $\mathcal{M}[\mathbf{m}]$ to construct effective energy corrections to classical kinetic equations. (Heitzinger, Nedjalkov, Vasileska, CR).

MULTI SCALE QUANTUM CORRECTIONS TO MC METHODS



- Oxide thickness = 1.2 nm
- Channel length = 25 nm
- Source/Drain length = 50 nm
- Channel width = 0.5 μm
- Junction depth = 30 nm
- Substrate thickness = 64 nm
- Substrate doping: $N_A=10^{19}$ cm^{-3}
- Doping of the source-drain regions: $N_D = 10^{19}$ cm^{-3}

- Idea: Approximate quantum effects by using a classical transport picture with a modified energy ($\longrightarrow$ modified particle trajectories).
- Compute effective energy by minimizing entropy for a given density function.

Algorithm

- Given $f(x, \xi, t) = \sum_n \delta(x - y_n)\delta(\xi - u_n)$

- Compute $n(x, t) = \int f(x, \xi, t)\, d\xi$ by a cloud in cell method.

- Compute $f_{equ}^{loc} = \mathcal{M}[n]$: the entropy minimizer for the particle density $n(x, t)$.

$$f_{equ}^{loc}(x, \xi) = D\mathcal{E}xp(\mathcal{E})(1 \cdot \lambda(x)), \quad n(x) = \int f_{equ}^{loc}(x, \xi)\, d\xi$$

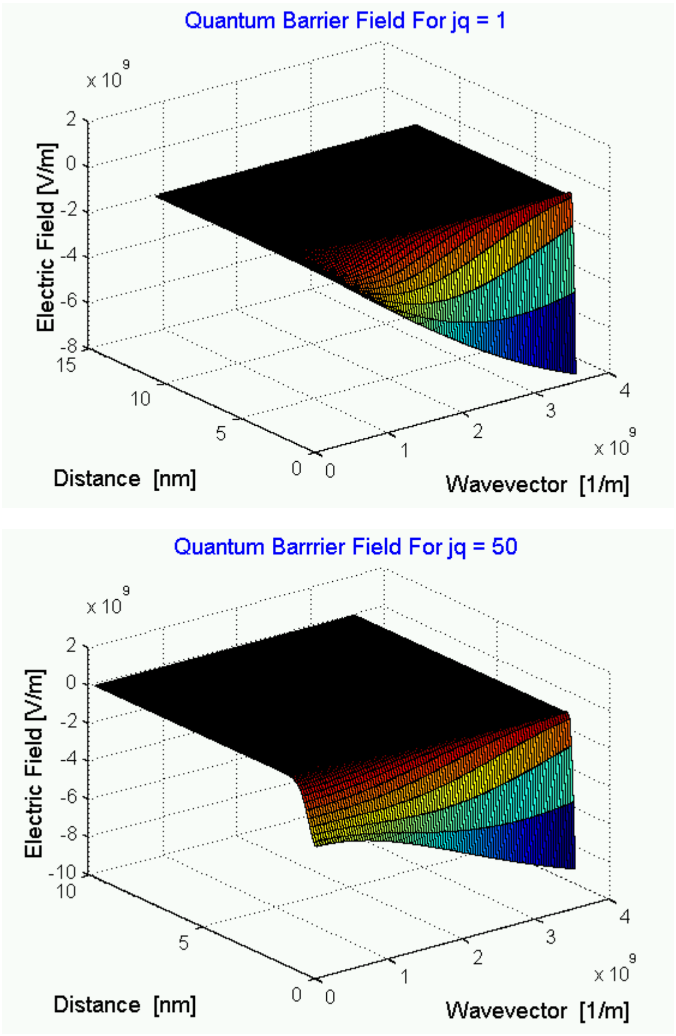
- Compute the effective energy $\boxed{\mathcal{E}_{eff} = \frac{\mathcal{E}(x,\xi) \circ f_{equ}^{loc}}{f_{equ}^{loc}}}$

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

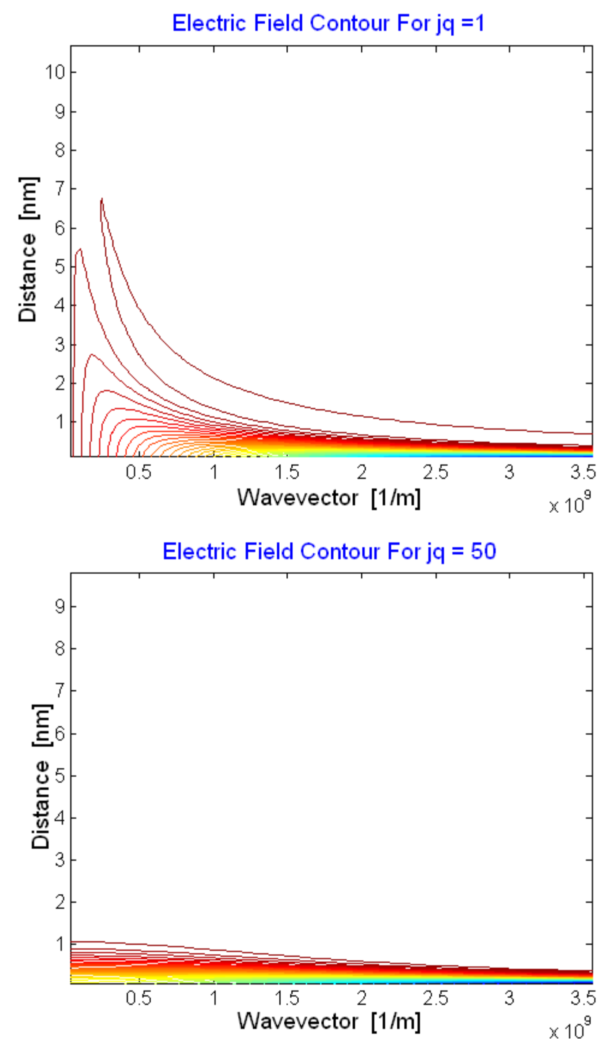
Remarks:

- Given $f_{equ}^{loc} = \mathcal{M}[n]$, the effective potential $\mathcal{E}^{eff}$ can be computed efficiently using FFTs.

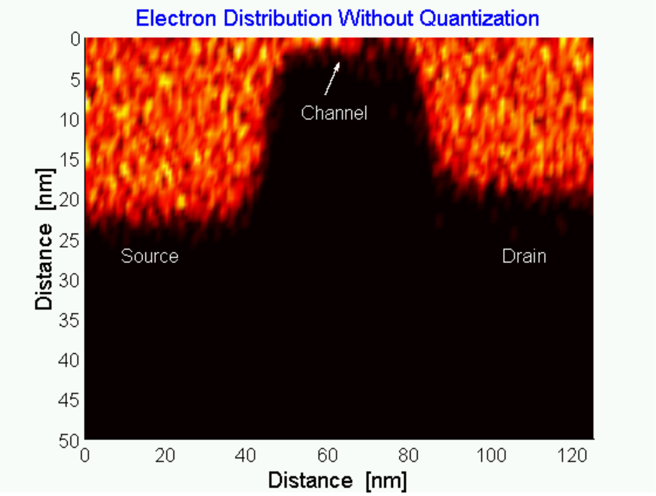
- Incorporate nonlocal effects, due to discontinuous confinement.

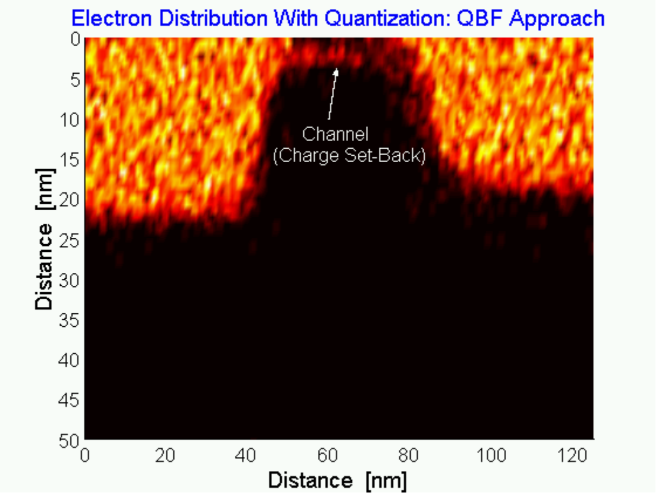


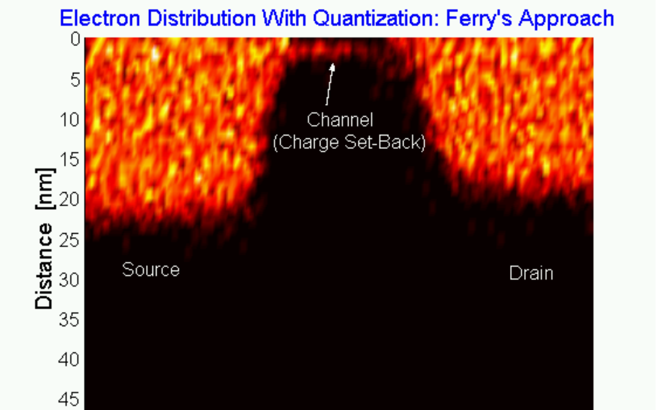
Effective force for a step

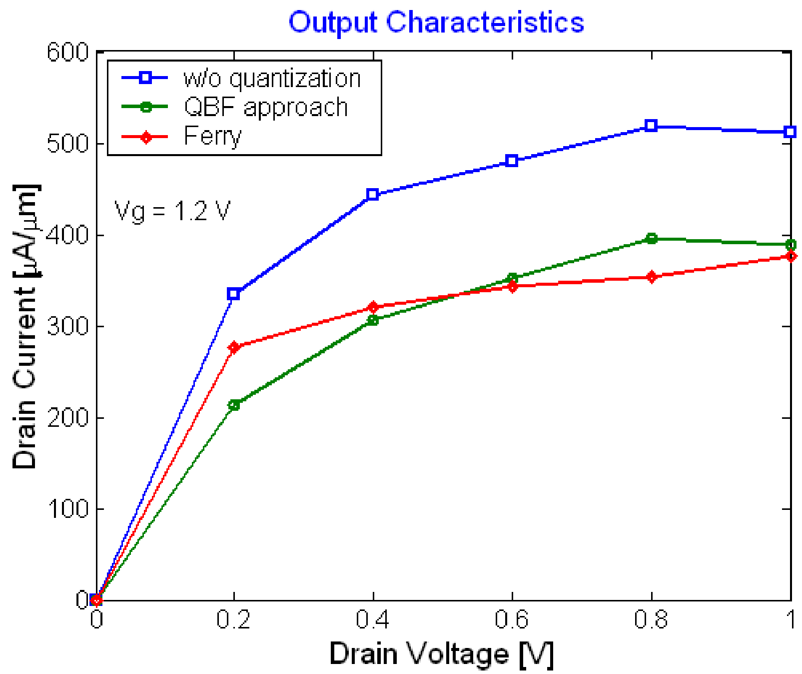


Effective force for a step


Electron Distribution Without Quantization
Channel
Source
Drain
Distance [nm]
Distance [nm]
0
5
10
15
20
25
30
35
40
45
50
0
20
40
60
80
100
120


Electron Distribution With Quantization: QBF Approach
Channel
(Charge Set-Back)
Distance [nm]
Distance [nm]
0
5
10
15
20
25
30
35
40
45
50
0
20
40
60
80
100
120


Electron Distribution With Quantization: Ferry's Approach
Channel
(Charge Set-Back)
Source
Drain
Distance [nm]
0
5
10
15
20
25
30
35
40
45



Output Characteristics
w/o quantization
QBF approach
Ferry
Vg = 1.2 V
Drain Current [μA/μm]
Drain Voltage [V]
0
100
200
300
400
500
600
0
0.2
0.4
0.6
0.8
1