Entropy Based Numerical Kinetics and Quantum Mechanical Corrections

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INTRODUCTION

$\longrightarrow$ Numerical methods for kinetic equations.

$\longrightarrow$ Dynamics given by competition between a Hamiltonian operator (free streeming, conservative) and a dissipative operator (collisions, diffusion).

f : density of particles with position x and momentum p

$$\partial_t f + C[\mathcal{E}, f] + Q[f], = 0$$

C : commutator with an energy function $\mathcal{E}(x,p)$. $\mathcal{E}$ is conserved along trajectories. (ballistic transport).

Q : Collision operator collisions of particles with each other and / or a background (thermalization - diffusion). $\mathcal{E}$ is dissipated by Q.

The classical commutator:

$$C[\mathcal{E}, f] = \nabla_x \cdot [\nabla_p \mathcal{E} f] - \nabla_p \cdot [\nabla_x \mathcal{E} f], \quad \mathcal{E}(x,p) = V(x) + \varepsilon(p)$$

V : potential energy, $\varepsilon(p)$: kinetic energy (vacuum: $\varepsilon(p) = \frac{|p|^2}{2}$, crystals: $\varepsilon(p)$ = band energy).

The collision operator:

$$Q(f) = \int f(x,p)K(x',p',x,p,f) - K(x,p,x',p',f)f(x',p')\,dx'p'$$

K : probability that state x', p' changes into state x, p due to a collision (with another particle or the background) $\times$ the collision frequency.

DISSIPATION AND ENTROPY

There is a convex functional $S(f) : \mathcal{B} \longrightarrow \mathbb{R}$, such that S is decreased by the collisions Q.

$$\partial_t f + Q[f] = 0 \;\Rightarrow\; \partial_t S(f) \leq 0$$

$-S(f)$ is the physical entropy.

Convexity:

$$S(\alpha f + (1-\alpha)g) \leq \alpha S(f) + (1-\alpha)S(g), \; \forall f, g$$

Dissipation:

$$DS(f)(Q[f]) \leq 0, \; \forall f,$$

- A numerical method for the solution of the Boltzmann equation should exhibit this dissipation property.
- This gives stability and well posedness.
- Numerical methods for macroscopic approximations (fluid dynamics, moment closures) should be based on the underlying kinetic structure.

OUTLINE $_6$

- Moment closures and Galerkin approximations. Leads to fluid equations, Levermore closures, and deterministic numerical methods for the BTE.
- Space - time discretizations:

  $\longrightarrow$ Preserve entropy structures on the discrete level.

  $\longrightarrow$ Examples: Energy transport equations, spherical harmonics expansions of the BTE.

  $\longrightarrow$ Applications: Charged particle transport in crystals.
- Quantum corrections and particle methods.

THE ENTROPY STRUCTURE

$\longrightarrow$ The collisions Q dissipate the entropy S. This means, we have $DS(f)(Q(f)) \geq 0 \, \forall f$.

$\longrightarrow$ $DS(f)(*)$ is a linear operator $\mathcal{B} \longrightarrow \mathbb{R}^+$. Can be written in terms of an integral kernel $h[f]$.

$$DS(f)(g) = \int h[f](x,p)g(x,p)\, dxp, \ \forall f, g$$

with $h[f]$ the entropy production rate.

$\longrightarrow$ This defines the nonlinear version of a scalar product.

$$\langle f, g \rangle = DS(f)(g) = \int h[f] g \, dxp$$

We have entropy dissipation of the collisions and entropy conservation of the Hamiltonian because of trace cylclicity.

$$\langle f, Q(f)\rangle \geq 0, \quad \langle f, C[\mathcal{E}, f]\rangle = 0 \Rightarrow \langle f, \partial_t f\rangle = \partial_t S(f) \leq 0$$

Dynamics:

$S(f)$ decreases until it reaches its minimum given by $S(f) = \min \iff Q(f) = 0$.

Boltzmann's H- theorem. Information theory: Incremental knowledge gain by observing one experiment.

$$S(f,\mathcal{E}) = \int f(\ln f - 1 + c\mathcal{E}), \quad h[f,\mathcal{E}] = \ln(f) + c\mathcal{E}$$

For $c \neq 0$ this is a relative entropy

MOMENT EQUATIONS - MAXIMUM LIKELIHOOD CLOSURES

$\longrightarrow$ Galerkin approximation of the transport equation

$\longrightarrow$ Choose test functions $\kappa_z(x,p)$ and define

$$m_z(t) = \int \kappa_z(x,p) f(x,p,t)\, dxp \;\Rightarrow$$

$$\partial_t m_z + F_z + q_z = 0$$

$$F_z = \int \kappa_z C[\mathcal{E},f]\, dxp, \quad q_z = \int \kappa_z Q(f)\, dxp$$

Examples

1. **Moment equations**

$$\kappa_{nr}(x,p) = \delta(x-r)p^{\otimes n},\ z = (n,r)$$

(hydrodynamics, Levermore closures).

2. **Spherical harmonics**

$$\kappa_{nru}(x,p) = \delta(x-r)\delta(\varepsilon(p)-u)\Gamma_n(\theta),\ z = (n,r,u),\ p = \varepsilon(p)p_0(\theta)$$

This leads to the closure problem of finding an ansatz for f as a function of the m_z.

The maximum likelihood closure

$\longrightarrow S(f)$ can e interpreted as the differential amount of information learned by making an observation of the system, governed by the probability distribution f.

$\longrightarrow$ Therefore, the most likely distribution f, given that we know $m_z\ \forall z$, is the solution of the constrained minimization problem

$$f = \phi(m_z), \quad S(\phi(m_z)) = \min\{S(f) : \int \kappa_z f \, dxp = m_z, \ \forall z\}$$

The solution to this problem is given in terms of Lagrange multiplyers μ_z

$$h[\phi(m_z)](x,p) = \sum_z \kappa_z(x,p)\mu_z,$$

$$\int \kappa_z(x,p)\phi(m_z)(x,p) \, dxp = m_z, \ \forall z$$

This gives the moment equations

$$\partial_t m_z + F(m_z) + q(m_z) = 0,$$

$$F(m_z) = \int \kappa_z C[\mathcal{E}, \phi] \, dxp,$$

$$h(\phi, \mathcal{E})(x,p) = \sum_z \kappa_z \mu_z, \quad \int \kappa_z \phi \, dxp = m_z, \, \forall z$$

Together with the nonlinear scalar product

$$\langle m, n \rangle = \int \mu n \, drp,$$

and the entropy equalities and inequalities

$$\langle m, F(m) \rangle = 0, \quad \langle m, q(m) \rangle \geq 0 \Rightarrow \langle m, \partial_t m \rangle = \partial_t s(m) \leq 0$$

for the entropy $s(m) = S(\phi)$ on the moment level.

Issues

- We have to be able to compute F and q.
- The involved integrals have to be finite.

Example I$_{16}$

Generalized hydrodynamics - (Levermore closures)

Particle - particle scattering $\Rightarrow$ classical entropy:

$$S(f) = \int f(\ln f - 1)\, dxp, \quad h(f) = \ln f,$$

Basis functions:

$$\kappa_{nr}(x,p) = \delta(x-r)\mathcal{P}_n(p), \quad z = (n,r)$$

$\mathcal{P}_n(p)$: vector polynomials.

Closure:

$$\phi(x,p) = \exp[\sum_{nr} \mathcal{P}_n(p)\mu_n(x)]$$

Moment realizability: $\mathcal{P}_n$ and μ_n have to be such that the moments actually are finite!

Simplest case: the compressible Euler equations $\mathcal{P}_n(p) = (1, p, |p|^2)$

$$\partial_t m_0 + \nabla_x \cdot m_1 = 0,$$

$$\partial_t m_1 + \nabla \cdot [m_0 T I + \frac{m_1 m_1^T}{m_0}] + \nabla V m_0 + q_1 = 0$$

$$\partial_t m_2 + \nabla \cdot [\frac{m_2}{m_0} m_1 + 2T m_1 - m_0 \nabla T)] + 2\nabla V \cdot m_1 + q_2 = 0$$

$3T := \frac{m_2}{m_0} - \frac{|m_1|^2}{m_0^2}$

Entropy:

$$s(m) = m_0[\ln(m_0) - \frac{3}{2}\ln(T) - \frac{|m_1|^2}{2m_0^2 T}] + \frac{|m_1|^2}{T m_0} - \frac{m_2}{T}$$

Example II

Spherical harmonics expansions with general S and h.

$\longrightarrow$ The energy kinetic ε is a free variable.

Test functions are

$$\kappa_{nru}(x,p) = \delta(x-r)\delta(\varepsilon(p)-u)\Gamma_n(\theta), \quad z=(n,r,u)$$

$$p = \varepsilon(p)p_0(\theta), \quad \varepsilon(p_0)=1, \quad \int f\,dp = \int f D(\varepsilon)\,d\varepsilon\theta$$

Closure:

$$\phi(x,p) = h^{-1}[\textstyle\sum_n \Gamma_n(\omega)\mu_n(x,\varepsilon(p))]$$

Relation between moments and entropy variables:

$$m_{nxu} = D(w)\int \Gamma_n(\omega)\exp[\textstyle\sum_m \Gamma_m(\omega)\mu_m(x,u)]\,d\omega$$

The resulting integrals are over angular variables only, and therefore always finite!

DISCRETIZATION METHODS (spatial)$_{21}$

Goal: Spatial discretization methods for the moment closure, preserving the entropy structure on the discrete level.

Example: Charged particle transport in transistors.

Features:

$\longrightarrow$ Heating

$\longrightarrow$ Non - equilibrium distributions and phenomena.

$\longrightarrow$ Quantum effects.

Moment equations:

$$\partial_t m + F + q = 0, \quad F_z = \int \kappa_z C[\mathcal{E}, \phi]\, dxp, \quad q_z = \int \kappa_z Q(\phi)\, dxp$$

moment - entropy variable relations:

$$\phi(x,p) = h^{-1}(\textstyle\sum_z \kappa_z(x,p)\mu_z), \quad \int \kappa_z \phi\, dxp = m_z\ \forall z$$
$$\langle m, n\rangle = \textstyle\sum_z \mu_z n_z$$

- The closure flux F conserves the entropy $\langle m, F\rangle = 0,\ \forall m$.
- The collision terms q dissipate the entropy $\langle m, q\rangle \geq 0,\ \forall m$.
- These relations should be maintained by the discretization.
- This is achieved by discretizing the closure flux F in weak form, using its adjoint under $\langle *, *\rangle$.

The commutator $C[\mathcal{E}, *]$ maps even into odd functions and vice versa.

Split the test function space into even and odd functions $\kappa_z = \left(\kappa_z^e, \kappa_z^o\right)$, and correspondingly, for moments and entropy variables

$m = (m^e, m^o)$, $\mu_z = (\mu_z^e, \mu_z^o)$

$$\partial_t m^e + F^e + q^e = 0, \quad \partial_t m^o + F^o + q^o = 0,$$

and $F^e, \ F^o$ conserve the entropy, i.e.

$$\langle m^e, F^e \rangle + \langle m^o, F^o \rangle = 0, \ \forall m^e, m^o$$

holds. This relation has to be maintained for any discretization.

We choose a conservative discretization of F^e and define F^o in a weak formulation as

$$\int \nu F^o(m^e)\, drp = \langle n, F^o(m^e)\rangle = -\langle m^e, F^e(m^e, n)\rangle,$$

ν : test function

$$\psi(x,p) = h^{-1}(\sum_z \kappa_z(x,p)\nu_z), \quad \int \kappa_z \psi \, dxp = n_z, \, \forall z$$

- This is possible if the odd part of the flux F^o does not depend on the odd moments m^o.
- This is the case in diffusive regimes, where $q^o >> q^e$ holds ($m^o \to \lambda m^o, \; \lambda^2 \approx \frac{q^e}{q^o}$).
- This is the case for linearized collision operators.

The energy transport equations $_{28}$

$$\lambda \partial_t m_0 + \lambda \nabla_x \cdot m_1 = 0,$$

$$\lambda^2 \partial_t m_1 + \nabla \cdot [m_0 T I + \lambda^2 \frac{m_1 m_1^T}{m_0}] + \nabla V m_0 + q_1 = 0$$

$$\lambda \partial_t m_2 + \nabla \cdot [\lambda \frac{m_2}{m_0} m_1 + 2\lambda T m_1)] + 2\lambda \nabla V \cdot m_1 + \lambda q_2 = 0$$

$$3T = \frac{m_2}{m_0} - \frac{\lambda^2 |m_1|^2}{m_0^2}$$

$$\partial_t m_0 + \nabla_x \cdot m_1 = 0,$$

$$\nabla \cdot [\frac{m_2}{3m_0} I] + \nabla V m_0 + q_1 = 0$$

$$\partial_t m_2 + \nabla \cdot [\lambda \frac{5m_2}{3m_0} m_1)] + 2\nabla V \cdot m_1 + q_2 = 0$$

$$3T = \frac{m_2}{m_0}$$

Entropy:

$$s(m) = m_0[\ln(m_0) - \frac{3}{2}\ln(T) - 1]$$

Discretize F^o as

$$\nabla \cdot [\frac{m_2}{3m_0} I] + V m_0 =$$
$$\frac{m_2}{3}\{\nabla[\ln m_0 - \frac{3}{2}\ln(2\pi T) + \frac{V}{T}] - (\frac{5}{2}T + V)\nabla[\frac{1}{T}]\}$$

A one dimensional model

FIGURE 1: Potential

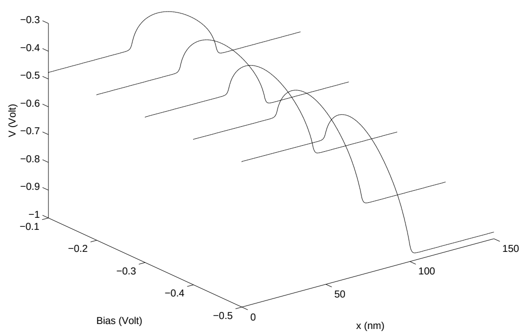
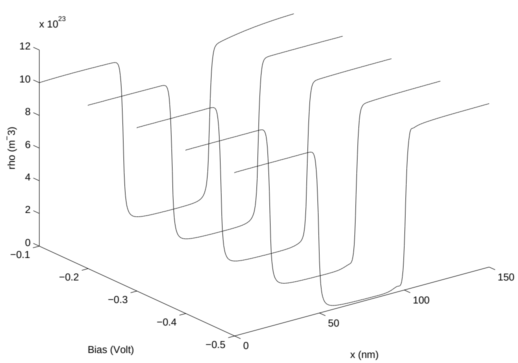


FIGURE 2: Particle Density



One dimensional simulation of the effective p-n-p diode using the energy transport equations.

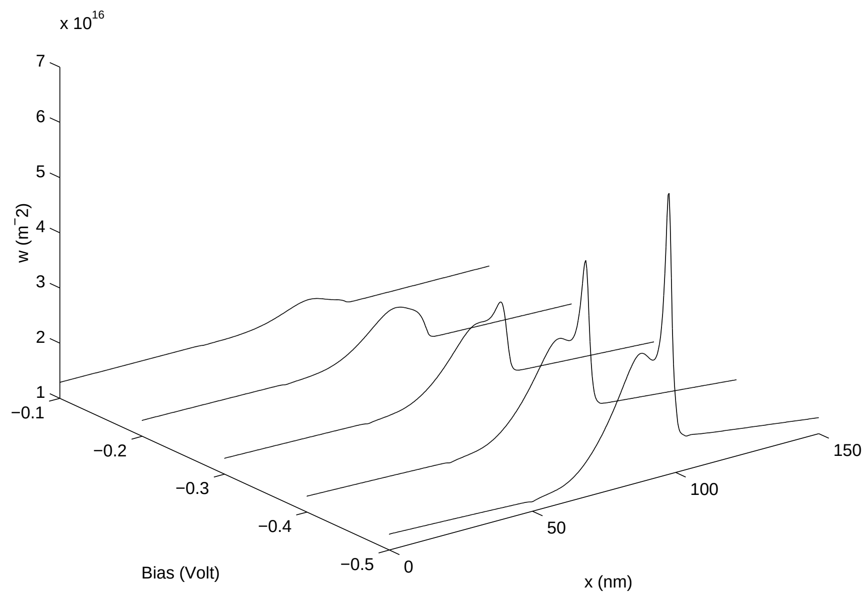
(Potential)

High velocity transport through the depleted channel.

(Carrier density)

Thermal energy

FIGURE 4: Energy Density



Kinetic energy of the carriers is transferred onto the thermal energy at the end of the depletion region.

Linear collisions

- Main collision mechanism is scattering with a background.
- In these collisions particles gain / loose an amount $\hbar\omega$ of energy.

$$\int \psi(p) Q(f)(x,p)\, dp =$$
$$\int [\psi(p) - \psi(p')] K(p,p') [e^{\mathcal{E}(x,p)} f(x,p) - e^{\mathcal{E}(x,p')} f(x,p')]\, dpp'$$
$$K(p,p') = \exp[-\tfrac{\mathcal{E}+\mathcal{E}'}{2}] \sum_{\sigma=\pm 1} \delta(\mathcal{E} - \mathcal{E}' + \sigma\hbar\omega)$$

Quadratic entropy

$$S(f) = \tfrac{1}{2} \int e^{\mathcal{E}} f^2\, dxp, \quad h(f) = e^{\mathcal{E}} f$$

SPHERICAL HARMONICS $_{34}$

Leave energy as a free variable. expand the angular components of p in spherical harmonics.

$$\kappa_{nru}(x,p) = \delta(r-x)\delta(\varepsilon(p)-u)\Gamma_n(\theta), \quad p = \varepsilon(p)p_0(\theta)$$

Expand in spherical harmonic basis functions.

Discretize F^e

$$F^e := C[\mathcal{E}, f^o] = \nabla_x \cdot [f^o \nabla_p \mathcal{E}] - \nabla_p \cdot [f^o \nabla_x \mathcal{E}]$$

in space via any conservative discretization. Discretize F^o as the negative dual of F^e under $\langle *, * \rangle$.

$$F^o = e^{-\mathcal{E}} \nabla_x (e^{\mathcal{E}} f^e) \cdot \nabla_p \mathcal{E} - e^{-\mathcal{E}} \nabla_p (e^{\mathcal{E}} f^e) \cdot \nabla_x \mathcal{E}$$

Kinetic density

FIGURE 5: r^2*f:,Bias=−0.4V,x=30.0752nm

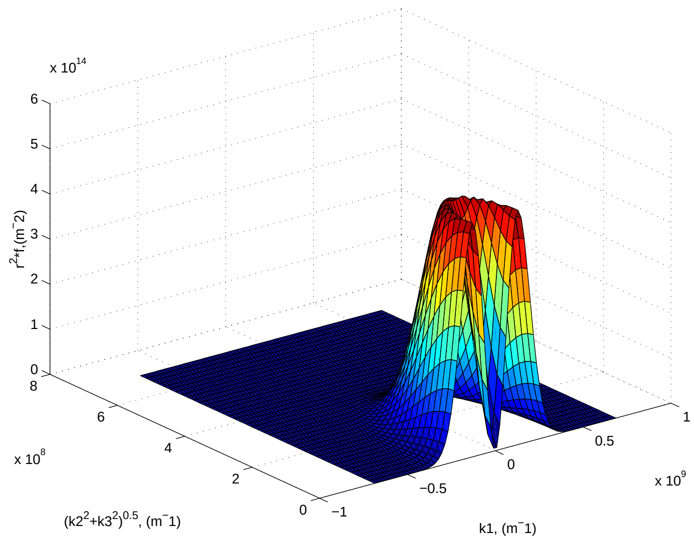
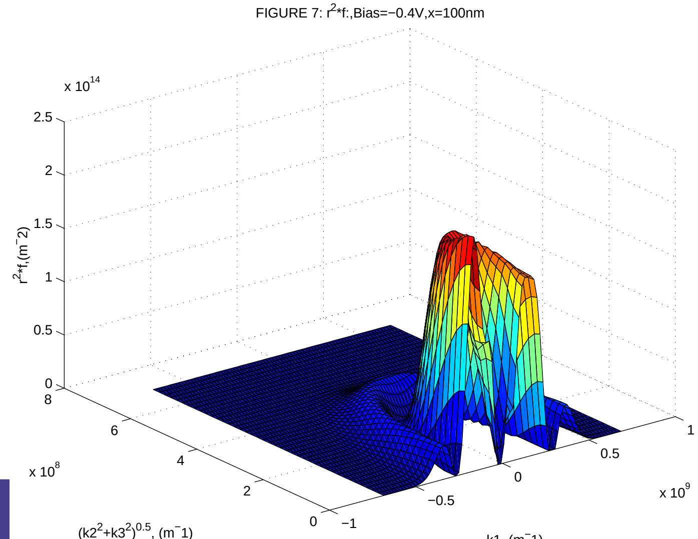


FIGURE 7: r^2*f:,Bias=−0.4V,x=100nm



-Plot $f\sqrt{2\varepsilon(p)}$ as a function of lateral momentum and radius.

- Essentially a Maxwellian outside the channel.

outside the channel

end of channel

$\longrightarrow$ High thermal energy not created by a broadening Maxwellian but by high energy tails.

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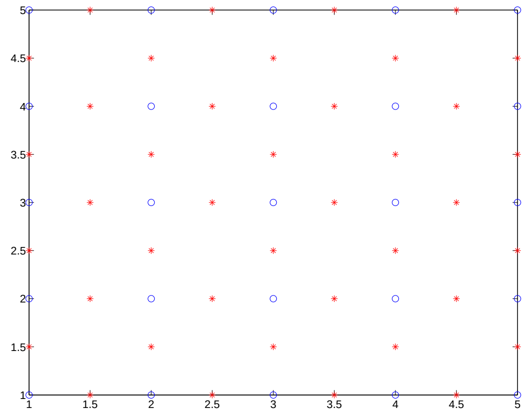
GRIDS



Box - grid: blue: density, red:flux

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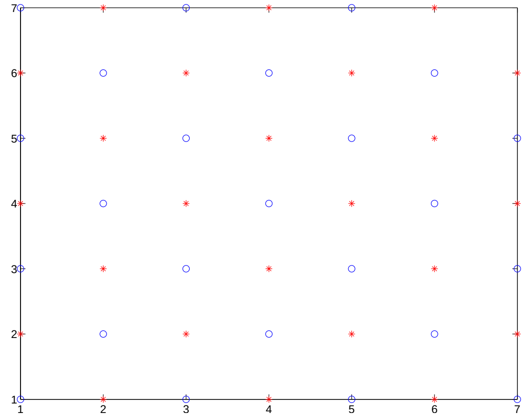
The flux moments m^o and the density moments m^e have to be defined on dual grids.



Staggered grid

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The definition of the operator via duality introduces a natural interpolation procedure.

TIME DISCRETIZATION $_{37}$

- Complicated mixture of ballistic transport, dispersive waves and diffusion (collisions).
- To compute the transient response accurately it is absolutely necessary to avoid artificial diffusion effects!
- Could be done by using ENO (Carrillo, Gamba, Shu).

$$\partial_t f^e + F^e + q^e = 0, \quad \partial_t f^o + F^o + q^o = 0, \quad F^o = -(F^e)^*$$

The Yi cell (Maxwell equations): Two operators, defined on dual grids whose product is self adjoint and negative semidefinite.

$$\frac{1}{\Delta t}(f^e_{n+1} - f^e_n) + F^e_n + q^e_{n+1} = 0, \quad \frac{1}{\Delta t}(f^o_{n+1} - f^o_n) + F^o_{n+1} + q^o_{n+1} = 0$$

Except for the collisions, this is an explicit scheme!

Numerical diffusion

In the absence of collisions the linearization of this reduces to

$$\frac{1}{\Delta t}(f^e_{n+1} - f^e_n) + L f^o_n = 0, \quad \frac{1}{\Delta t}(f^o_{n+1} - f^o_n) - L^* f^e_{n+1} = 0$$

Proposition

Without collisions, all the eigenvalues of the linearized scheme lie precisely on the unit circle.

$\Rightarrow$ no artificial diffusion.

'Mildly unstable': Without collisions, roundoff error effects would grow linearly.

QUANTUM CORRECTIONS $_{40}$

- To include quantum mechanical effects, we have to start from the Schrödinger equation for a mixed state, giving a density matrix ρ.
- Using the Wigner - Weyl transform, this can be transformed into a kinetic equation for the Wigner function which, formally, is an $O(\hbar^2)$ perturbation of the Boltzmann equation.
- The entropy S is replaced by the quantum entropy $S(\rho) = Tr[\rho(\ln(\rho) - 1)]$.

The Wigner - von Neumann equation

Given by the Schrödinger equation for the density matrix under the Wigner - Weyl transform.

For a density matrix $\rho(x, y, t)$ of a mixed state, we have

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

gives the Wigner equation:

$$\partial_t f + C_q[\mathcal{E}, f] + Q[f] = 0,$$

$$C_q[\mathcal{E}, f] = \nabla_x \cdot [\nabla_p \mathcal{E}_q f] - \nabla_p \cdot [\nabla_x \mathcal{E}_q f]$$

$\mathcal{E}_q$ is now an operator instead of a function, given, in pseudo differential operator notation, by

$$\mathcal{E}_q(x, p, \nabla_x, \nabla_p) = \frac{1}{2} \int_{-1}^{1} \mathcal{E}(x - \frac{sh}{2i}\nabla_p, p + \frac{sh}{2i}\nabla_x) \, ds$$

$\longrightarrow$ Traces of density matrices $\longrightarrow$ integrals in the Wigner picture.

The entropy in the Wigner picture is

$$S(f) = Tr[\rho(\ln r - 1)] = \int f(\mathcal{L}n f - 1)\, dxp,$$
$$\mathcal{L}n(f) = W(\ln(W^{-1} f))$$

$\mathcal{L}n(f)$ is the operator logarithm in the Wigner picture.

- The whole approach (maximum entropy - likelihood closures), conservation and dissipation of the entropy, etc. carries through, in principle, in the quantum picture
- All involved operators are nonlocal.
- Leads to quantum hydrodynamics (Degond, CR,03), quantum versions of the Levermore closures (Mehats, Gallego,04) and spherical harmonics solutions of the quantum Boltzmann equation (Degond, Mehats, CR,05).
- Because of the nonlocality, we want to adapt particle based methods to quantum kinetics, rather than moment closures.

QUANTUM COLLISIONS $_{46}$

$\longrightarrow$ The collisions act on entropy variables rather than on densities.

$\longrightarrow$ Replace only the relation between entropy variables and densities by the corresponding quantum relations.

The nonlinear relations: $h_c(f) = \ln(f), \quad h_q(f) = \mathcal{L}n(f)$

Linearized at $f = e^{-\mathcal{E}}$ and $f = \mathcal{E}xp(-\mathcal{E})$:

$$h_c(f) = e^{\mathcal{E}} f, \quad h_q(f) = D\mathcal{L}n(\mathcal{E}xp(-\mathcal{E}))(f) = D\mathcal{E}xp(-\mathcal{E})^{-1} f$$

Replace $Q_q(f) \;\rightarrow\; Q_c(h_c^{-1}(h_q(f))),$

Correct equilibrium and dissipation properties.

Equilibrium:

$$Q_q(f) = 0 \iff h_c^{-1}(h_q(f)) = \mathcal{E}xp(-\mathcal{E})$$
$$\iff f = \mathcal{E}xp(-\mathcal{E})$$

Entropy dissipation:

$$\int h_q(f)Q_q(f)\,dxp = \int h_c(g)Q_c(g)\,dxp \geq 0, \quad g = h_c^{-1}(h_q(f))$$

$h_q = D\mathcal{L}n(\mathcal{E}xp(-\mathcal{E}))$ computed as a (big!) scattering matrix.

EFFECTIVE POTENTIALS

Particle discretizaion of the quantum coomutator.

$$C_q[\mathcal{E}, f] = \nabla_x \cdot [\nabla_p \mathcal{E}_q f] - \nabla_p \cdot [\nabla_x \mathcal{E}_q f]$$
$$\mathcal{E}_q(x, p, \nabla_x, \nabla_p) = \frac{1}{2} \int_{-1}^{1} \mathcal{E}(x - \frac{sh}{2i}\nabla_p, p + \frac{sh}{2i}\nabla_x)\, ds$$

Write $\mathcal{E}_q$ in terms of an effective potential

$$\mathcal{E}_q(x, p, \nabla_x, \nabla_p) f = \mathcal{E}_{eff}(x, p, f) f$$

$\mathcal{E}_{eff}(x, p, f)$ computed for a given f by a cloud in cell method.

Incorporates nonlocal effects, due to discontinuous confinement very well.