Entropy Based Numerical Kinetics and Quantum Mechanical Corrections

Christian Ringhofer (Arizona State University)

joint work with:

P. Degond, F. Mehats (Toulouse), S. Ahmed, C. Gardner, D. Vasileska (ASU)
Numerical methods for kinetic equations.

Dynamics given by competition between a Hamiltonian operator (free streaming, 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 $S(f) : \mathcal{B} \rightarrow \mathbb{R}$, 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.
• Moment closures and Galerkin approximations. Leads to fluid equations, Levermore closures, and deterministic numerical methods for the BTE.

• Space - time discretizations:
  → Preserve entropy structures on the discrete level.
  → Examples: Energy transport equations, spherical harmonics expansions of the BTE.
  → Applications: Charged particle transport in crystals.

• Quantum corrections and particle methods.
→ The collisions $Q$ dissipate the entropy $S$. This means, we have

\[ DS(f)(Q(f)) \geq 0 \ \forall f. \]

→ $DS(f)(\ast)$ is a linear operator $\mathcal{B} \rightarrow \mathbb{R}^+$. 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.

→ 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 cyclicity.

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

**Dynamics:**

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

→ Galerkin approximation of the transport equation
→ Choose test functions \( \kappa_z(x, p) \) and define

\[ m_z(t) = \int \kappa_z(x, p)f(x, p, t) \, dx \, dp \quad \Rightarrow \]

\[ \partial_t m_z + F_z + q_z = 0 \]

\[ F_z = \int \kappa_z C[\mathcal{E}, f] \, dx \, dp, \quad q_z = \int \kappa_z Q(f) \, dx \, dp \]
Examples

1. Moment equations

\[ \kappa_{nr}(x, p) = \delta(x - r)p \otimes n, \quad z = (n, r) \]

(hydrodynamics, Levermore closures).

2. Spherical harmonics

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

This leads to the closure problem of finding an ansatz for \( f \) as a function of the \( m_z \).
The maximum likelihood closure

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

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

\[
f = \phi(m_z), \quad S(\phi(m_z)) = \min \{ S(f) : \int \kappa_z f \, dx_p = m_z, \forall z \}\]

The solution to this problem is given in terms of Lagrange multipliers \( \mu_z \)

\[
h[\phi(m_z)](x, p) = \sum_z \kappa_z(x, p)\mu_z, \\
\int \kappa_z(x, p)\phi(m_z)(x, p) \, dx_p = m_z, \forall z
\]
This gives the moment equations

\[ \partial_t m_z + F(m_z) + q(m_z) = 0, \]
\[ F(m_z) = \int \kappa_z C[\mathcal{E}, \phi] \, dxp, \]
\[ h(\phi, \mathcal{E})(x, p) = \sum_z \kappa_z \mu_z, \quad \int \kappa_z \phi \, dxp = m_z, \quad \forall z \]

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.
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:

\[
\kappa_{nr}(x, p) = \delta(x - r)P_n(p), \quad z = (n, r)
\]

\( P_n(p) \): vector polynomials.

Closure:

\[
\phi(x, p) = \exp\left[\sum_{nr} P_n(p)\mu_n(x)\right]
\]

Moment realizability: \( P_n \) and \( \mu_n \) have to be such that the moments actually are finite!
Simplest case: the compressible Euler equations $P_n(p) = (1, p, |p|^2)$

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

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

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

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

Entropy:

$$s(m) = m_0 [\ln(m_0) - \frac{3}{2} \ln(T) - \frac{|m_1|^2}{2m_0^2 T}] + \frac{|m_1|^2}{Tm_0} - \frac{m_2}{T}$$
Spherical harmonics expansions with general $S$ and $h$.

$\rightarrow$ The energy kinetic $\varepsilon$ 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:

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

Relation between moments and entropy variables:

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

The resulting integrals are over angular variables only, and therefore always finite!
Goal: Spatial discretization methods for the moment closure, preserving the entropy structure on the discrete level.
Example: Charged particle transport in transistors.
Features:
→ Heating
→ Non-equilibrium distributions and phenomena.
→ Quantum effects.
Moment equations:
\[ \partial_t m + F + q = 0, \quad F_z = \int \kappa_z C[\mathcal{E}, \phi] \, dp, \quad q_z = \int \kappa_z Q(\phi) \, dp \]

moment - entropy variable relations:
\[ \phi(x, p) = h^{-1}(\sum_z \kappa_z(x, p)\mu_z), \quad \int \kappa_z \phi \, dp = m_z \forall z \]

- 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 $C[\mathcal{E}, \ast]$ maps even into odd functions and vice versa.

Split the test function space into even and odd functions $\kappa_z = (\kappa^e_z, \kappa^o_z)$, and correspondingly, for moments and entropy variables $m = (m^e, m^o)$, $\mu_z = (\mu^e_z, \mu^o_z)$

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

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

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

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

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

$\nu$ : 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
  $$\left(m^o \rightarrow \lambda m^o, \lambda^2 \approx \frac{q^e}{q^o}\right).$$
- This is the case for linearized collision operators.
The energy transport equations

\[\lambda \partial_t m_0 + \lambda \nabla_x \cdot m_1 = 0,\]
\[\lambda^2 \partial_t m_1 + \nabla \cdot [m_0 TI + \lambda^2 \frac{m_1 m_1^T}{m_0}] + \nabla V m_0 + q_1 = 0\]
\[\lambda \partial_t m_2 + \nabla \cdot [\lambda \frac{m_2}{m_0} m_1 + 2\lambda T m_1)] + 2\lambda \nabla V \cdot m_1 + \lambda q_2 = 0\]

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

\[\partial_t m_0 + \nabla_x \cdot m_1 = 0,\]
\[\nabla \cdot \left[ \frac{m_2}{3m_0} I \right] + \nabla V m_0 + q_1 = 0\]
\[\partial_t m_2 + \nabla \cdot \left[ \lambda \frac{5m_2}{3m_0} m_1 \right] + 2\nabla V \cdot m_1 + q_2 = 0\]

\[3T = \frac{m_2}{m_0}\]

Entropy:

\[s(m) = m_0[\ln(m_0) - \frac{3}{2} \ln(T) - 1]\]
Discretize $F^o$ as

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

$$\frac{m_2}{3} \left\{ \nabla \left[ \ln m_0 - \frac{3}{2} \ln (2\pi T) + \frac{V}{T} \right] - \left( \frac{5}{2} T + V \right) \nabla \left[ \frac{1}{T} \right] \right\}$$
A one dimensional model

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)
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.

\[
\int \psi(p)Q(f)(x, p) \, dp = \int [\psi(p) - \psi(p')]K(p, p')[e^{\mathcal{E}(x,p)}f(x, p) - e^{\mathcal{E}(x,p')}f(x, p')] \, dpdp'
\]

\[
K(p, p') = \exp[-\frac{\mathcal{E} + \mathcal{E}'}{2}] \sum_{\sigma = \pm 1} \delta(\mathcal{E} - \mathcal{E}' + \sigma \hbar \omega)
\]

Quadratic entropy

\[
S(f) = \frac{1}{2} \int e^\mathcal{E} f^2 \, dxp, \quad h(f) = e^\mathcal{E} f
\]
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 \( F^e \)

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

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

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

- Essentially a Maxwellian outside the channel.

\[ k_1, (m^{-1}) \]

\[ r_2^*f, Bias=-0.4V, x=30.0752nm \]

outside the channel

\[ r_2^*f, (m^{-2}) \]

end of channel

\[ \rightarrow \] High thermal energy not created by a broadening Maxwellian but by high energy tails.
Box - grid: **blue**: density, **red**: flux

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

Staggered grid

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

\[
\frac{1}{\Delta t}(f_{n+1}^e - f_n^e) + L f_n^o = 0, \quad \frac{1}{\Delta t}(f_{n+1}^o - f_n^o) - L^* f_{n+1}^e = 0
\]

Proposition

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

\[\Rightarrow \text{no artificial diffusion.}\]

'Mildly unstable': Without collisions, roundoff error effects would grow linearly.
• To include quantum mechanical effects, we have to start from the Schrödinger equation for a mixed state, giving a density matrix $\rho$.

• 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

$$\mathcal{E}_q(x, p, \nabla_x, \nabla_p) = \frac{1}{2} \int_{-1}^{1} \mathcal{E}(x - \frac{s\hbar}{2i} \nabla_p, p + \frac{s\hbar}{2i} \nabla_x) \, ds$$
Traces of density matrices → 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.
→ The collisions act on entropy variables rather than on densities.
→ 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:

\[ Q_q(f) = 0 \iff h_c^{-1}(h_q(f)) = \exp(-\mathcal{E}) \iff f = \exp(-\mathcal{E}) \]

Entropy dissipation:

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

\[ h_q = D \mathcal{L} \ln(\exp(-\mathcal{E})) \] computed as a (big!) scattering matrix.
EFFECTIVE POTENTIALS

Particle discretization of the quantum commutator.

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

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

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.