Quantum Hydrodynamics models derived from the entropy principle

P. Degond[1], Ch. Ringhofer[2]

[1] MIP, CNRS and Université Paul Sabatier,

118 route de Narbonne, 31062 Toulouse cedex, France

degond@mip.ups-tlse.fr http://mip.ups-tlse.fr

[2] Dep. of Math., Arizona State University,

Tempe, Arizona 85287-1804, USA

ringhofer@asu.edu http://math.la.asu.edu/ chris/

Summary

1. Introduction

Introduction

	Classical	Quantum
Microscopic models	Boltzmann eq.	Quantum Liouville eq.
Macroscopic models	Fluid mech. eqs.	(?) special cases: Bohmian mech. (1 particle) perturbative ext. to many-particle

2. Review of classical hydrodynamic theories

Microscopic vs macroscopic models

- Microscopic models: phase-space distribution function $f(x, p, t)$
- Boltzmann equation

$$\partial_t f + p \cdot \nabla_x f - \nabla_x V \cdot \nabla_p f = Q(f)$$

- Macroscopic models:
  - density $n(x, t)$
  - mean velocity $u(x; t)$
  - temperature $T(x, t)$

Balance equations (Euler eq.)

$$\frac{\partial}{\partial t}\begin{pmatrix} n \\ nu \\ n|u|^2 + 3nT \end{pmatrix} + \nabla_x \cdot \begin{pmatrix} nu \\ nuu + nT\,\mathrm{Id} \\ (n|u|^2 + 5nT)u \end{pmatrix} = \begin{pmatrix} 0 \\ -n\nabla_x V \\ -nu \cdot \nabla_x V \end{pmatrix}$$

- Euler eqs of gas dynamics.
  Pressure $= nT$: perfect gas Equation-of-State

- How to relate macroscopic models to microscopic eq. ?

Moment method

➠ n, $q = nu$, $2W = n|u|^2 + 3nT$ are moments of f:

$$\begin{pmatrix} n \\ q \\ 2W \end{pmatrix} = \int f \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} dp$$

Moment method

- Natural idea: (i) multiply Boltzmann eq. by 1, p, $|p|^2$ and integrate w.r.t. p:

$$\int (\partial_t f + p \cdot \nabla_x f - \nabla_x V \cdot \nabla_p f - Q(f)) \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} dp = 0$$

- (ii) use conservations:

$$\int Q(f) \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} dp = 0$$

Moment method (cont)

- (iii) Get conservation eqs

$$\frac{\partial}{\partial t}\begin{pmatrix} n \\ q \\ 2W \end{pmatrix} + \nabla_x \cdot \int f \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} p\, dp = \begin{pmatrix} 0 \\ -n\nabla_x V \\ -nu \cdot \nabla_x V \end{pmatrix}$$

- Problem: Express fluxes in term of the conserved variables $n,\ q,\ W$
  - $\int f p_i p_j \, dp$ (for $i \neq j$) and $\int f |p|^2 \, p\, dp$ cannot be expressed in terms of $n,\ q,\ W$.

- conservation eqs are not closed

Entropy minimization (Gibbs, Levermore)

- Closure: replace f by a solution of the entropy minimization problem:
- Let $n, T \in \mathbb{R}_+$, $u \in \mathbb{R}^3$ fixed. Find

$$\min\{H(f) = \int f(\ln f - 1) dp \text{ s.t.}$$

$$\int f \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} dp = \begin{pmatrix} n \\ nu \\ n|u|^2 + 3nT \end{pmatrix} \}$$

Entropy minimization (cont)

- Entropy minimization problem has solution:

$$M_{n,u,T} = \frac{n}{(2\pi T)^{3/2}} \exp\left(-\frac{|p-u|^2}{2T}\right)$$

- Maxwellian satisfies

$$\int M_{n,u,T} \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} dp = \begin{pmatrix} n \\ nu \\ n|u|^2 + 3nT \end{pmatrix}$$

- Gives the Euler eqs. of gas dynamics
  Levermore closures if more moments are retained

Quantum case

- Idea: use the same idea for quantum models.
- Not so simple ...

3. Quantum setting: basics

Density operator

- Basic object: ρ: Hermitian, postive, trace-class operator on $L^2(\mathbb{R}^d)$ s.t.

$$\mathrm{Tr}\rho = 1$$

- Typically:

$$\rho\psi = \sum_{s\in S} \rho_s(\psi, \phi_s)\, \phi_s$$

for a complete orthonormal system $(\phi_s)_{s\in S}$ and real numbers $(\rho_s)_{s\in S}$ such that $0 \leq \rho_s \leq 1$, $\sum \rho_s = 1$

Quantum Liouville equation

- $$i\hbar\partial_t\rho = [\mathcal{H}, \rho] + Q(\rho)$$

- $\mathcal{H}$ = Hamiltonian:

$$\mathcal{H}\psi = -\frac{\hbar^2}{2}\Delta\psi + V(x,t)\psi$$

- $Q(\rho)$ unspecified: accounts for dissipation mechnisms

Wigner Transform

- $\underline{\rho}(x, x')$ integral kernel of ρ:

$$\rho\psi = \int \underline{\rho}(x, x')\psi(x')\, dx'$$

- $W[\rho](x, p)$ Wigner transform of ρ:

$$W[\rho](x, p) = \int \underline{\rho}(x - \frac{1}{2}\xi, x + \frac{1}{2}\xi)\, e^{i\frac{\xi \cdot p}{\hbar}}\, d\xi$$

Inverse Wigner transform (Weyl quantization)

- Let $w(x,p)$. $\rho = W^{-1}(w)$ is the operator defined by:

$$W^{-1}(w)\psi = \frac{1}{(2\pi)^d} \int w(\frac{x+y}{2}, \hbar k)\, \psi(y) e^{ik(x-y)}\, dk\, dy$$

w= Weyl symbol of ρ.

- Isometries between $\mathcal{L}^2$ (Operators s.t. $\rho\rho^\dagger$ is trace-class) and $L^2(\mathbb{R}^{2d})$:

$$\mathrm{Tr}\{\rho\sigma^\dagger\} = \int W[\rho](x,p)\overline{W[\sigma](x,p)}\, \frac{dx\, dp}{(2\pi\hbar)^d}$$

Wigner equation

- Eq. for $w = W[\rho]$:

$$\partial_t w + p \cdot \nabla_x w + \Theta^\hbar[V]w = Q(w)$$

$$\Theta^\hbar[V]w = -\frac{i}{(2\pi)^d \hbar} \int (V(x + \frac{\hbar}{2}\eta) - V(x - \frac{\hbar}{2}\eta)) \times w(x, q)\, e^{i\eta\cdot(p-q)}\, dq\, d\eta$$

- $\Theta^\hbar[V]w \xrightarrow{\hbar \to 0} -\nabla_x V \cdot \nabla_p w$
- $Q(w)$ collision operator (unspecified)

4. Review of quantum hydrodynamic theories

1-particle quantum hydrodynamics

➠ Single state ψ

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2}\Delta\psi + V(x,t)\psi$$

Decompose

$$\psi = \sqrt{n}e^{iS/\hbar}$$

and define $u = \nabla_x S$. Then take real and imaginary parts

$$\partial_t n + \nabla_x \cdot nu = 0$$

$$\partial_t S + \frac{1}{2}|\nabla S|^2 + V - \frac{\hbar^2}{2}\frac{1}{\sqrt{n}}\Delta\sqrt{n} = 0$$

1-particle QHD (cont)

- Take ∇ of the phase eq.

$$\partial_t n + \nabla_x \cdot nu = 0$$
$$\partial_t u + u \cdot \nabla_x u = -\nabla_x (V + V_B)$$
$$V_B = -\frac{\hbar^2}{2} \frac{1}{\sqrt{n}} \Delta \sqrt{n}$$

V_B = Bohm potential

- Pressureless Gas dynamics w. additional Bohm potential term, of order $O(\hbar^2)$

Many-particle case

- Procedure:
  - Start w. statistical state, i.e. density operator
  - Average over the probabilities ρ_s
    $\Longrightarrow$ Closure problem

- Closure strategies:
  - Fourier law for the heat flux [Gardner]
  - Small temperature [Gasser, Markowich, Ringhofer]
  - Chapman-Enskog expansion [Gardner, Ringhofer]
  - Entropy minimization [D. ,Ringhofer]

5. QHD via entropy minimization

Moments

- Defined as in classical mechanics: Moments of the Wigner distribution

- List of monomials $\mu_i(p)$ e.g. $(1, p, |p|^2)$

$$\mu(p) = (\mu_i(p))_{i=0}^{N}$$

- $w(x,p) \longrightarrow$ moments $m[w] = (m_i[w])_{i=0}^{N}$

$$m_i[w] = \int w(x,p)\, \mu_i(p)\, dp$$

e.g. $m = (n, q, W)$

Moment method

- Take moments of the Wigner equation:

$$\partial_t m[w] + \nabla_x \cdot \int w \, \mu \, p \, dp + \int \Theta[V] w \, \mu \, dp = \int Q(w) \, \mu \, dp$$

- Assume conservations

$$\int Q(w) \, \mu \, dp = 0$$

- Closure problem: find an expression of the integrals at the l.h.s.

Entropy minimization principle

- Entropy:

$$H[\rho] = \mathrm{Tr}\{\rho(\ln\rho - 1)\} \quad ; \quad \rho = W^{-1}(w)$$

- Given a set of moments $m = (m_i(x))_{i=0}^{N}$, minimize $H(\rho)$ subject to the constraint that

$$\int W[\rho](x,p)\,\mu(p)\,dp = m(x) \quad \forall x$$

- Problem: express the moment constraints in terms of ρ

Moments in terms of ρ

- Dualize the constraint: Let $\lambda(x) = (\lambda_i(x))_{i=0}^N$ be an arbitrary (vector) test function

$$\int w(x,p)\,\mu(p)\lambda(x)\,\frac{dx\,dp}{(2\pi\hbar)^d} = \int m(x)\cdot\lambda(x)\,\frac{dx}{(2\pi\hbar)^d}$$

$$\mathrm{Tr}\{\rho\,W^{-1}[\mu(p)\cdot\lambda(x)]\} = \int m(x)\cdot\lambda(x)\,\frac{dx}{(2\pi\hbar)^d}$$

Entropy minimization principle: expression

- Given a set of (physically admissible) moments $m = (m_i(x))_{i=0}^N$, solve

$$\min\{\ H[\rho] = \mathrm{Tr}\{\rho(\ln\rho - 1)\} \quad \text{subject to:}$$

$$\mathrm{Tr}\{\rho\, W^{-1}[\mu(p)\cdot\lambda(x)]\} = \int m\cdot\lambda \frac{dx}{(2\pi\hbar)^d}$$

$$\forall\lambda = (\lambda_i(x))_{i=0}^N \quad \}$$

Solution of the entropy problem

- Solution is ρ_α,

$$\rho_\alpha = \exp(W^{-1}[\alpha(x) \cdot \mu(p)])$$

$\alpha = (\alpha_i(x))_{i=0}^N$ is determined s.t. $m[\rho_\alpha] = m$

- $$w_\alpha = W[\rho_\alpha] = \mathcal{E}\text{xp}(\alpha(x) \cdot \mu(p))$$

$$\mathcal{E}\text{xp}\, w = W[\exp(W^{-1}(w))]$$

(Quantum exponential)

- Analogy with the classical case $M_\alpha = \exp(\alpha \cdot \mu)$

Quantum moment models

- Take moments of the Wigner eq. and close with the quantum Maxwellian:

$$\partial_t \int \mathcal{E}\text{xp}(\alpha \cdot \mu)\, \mu \, dp + \nabla_x \cdot \int \mathcal{E}\text{xp}(\alpha \cdot \mu)\, \mu \, p \, dp$$
$$+ \int \Theta[V] \mathcal{E}\text{xp}(\alpha \cdot \mu)\, \mu \, dp = 0$$

- Provides an evolution system for the vector function $\alpha(x, t)$

Entropy

- Kinetic entropy $H[\rho]$ in terms of $w = W[\rho]$:

$$H[\rho] = \mathrm{Tr}\{\rho(\ln(\rho - 1)\} = \int w(\mathcal{L}\mathrm{n}\, w - 1)\frac{dx\, dp}{(2\pi\hbar)^d}$$

with quantum log: $\mathcal{L}\mathrm{n}\, w = W[\ln(W^{-1}(w))]$

- Fluid entropy $S(m)$:

$$S(m) = H[\rho_\alpha] = \int \mathcal{E}\mathrm{xp}(\alpha \cdot \mu)((\alpha \cdot \mu) - 1)\frac{dx\, dp}{(2\pi\hbar)^d}$$

where α is s.t. $\int \mathcal{E}\mathrm{xp}(\alpha \cdot \mu)\mu dp = m$

Entropy (cont)

- $S(m)$ convex
  Define: $\Sigma(\alpha)$, Legendre dual of S

- Inversion of the mapping $\alpha \to m$:

$$\frac{\delta S}{\delta m} = \alpha \, , \qquad \frac{\delta \Sigma}{\delta \alpha} = m$$

- Moment models compatible with the entropy dissipation

$$\partial_t S(m(t)) \leq 0$$

for any solution $m(t)$ of the QHD equations

Quantum Hydrodynamics

➟ $\mu = \{1, p, |p|^2\}$

$$\partial_t n + \nabla_x \cdot nu = 0$$
$$\partial_t nu + \nabla_x (nuu + \mathbb{P}) = -n \nabla_x V$$
$$\partial_t W + \nabla_x \cdot (Wu + \mathbb{P}u + \mathbb{Q}) = -nu \cdot \nabla_x V$$

➟ with $\mathbb{P}$ = pressure tensor, $\mathbb{Q}$ = heat flux:

$$\mathbb{P} = \int \mathcal{E}\mathrm{xp}(\alpha \cdot \mu)(p-u)(p-u) dp$$
$$2\mathbb{Q} = \int \mathcal{E}\mathrm{xp}(\alpha \cdot \mu)|p-u|^2 (p-u) dp$$

Quantum Hydrodynamics (cont)

- and

$$\alpha \cdot \mu = A + B \cdot p + C|p|^2$$

s.t.

$$\int \mathcal{E}\mathrm{xp}(\alpha \cdot \mu)\mu dp = (n, nu, W)^{Tr}$$

6. Quantum collision operators

Classical Boltzmann operator

$$Q(w) = \int B(|p - p_1|, \Omega)(w' w_1' - w w_1) dp_1 \, d\Omega$$

$$p + p_1 = p' + p_1' \qquad p^2 + p_1^2 = {p'}^2 + {p'}_1^2$$

$\Omega \in \mathbb{S}^2$ scattering angle; B scattering cross-section

- Preserves mass, momentum and energy locally
- Kernel $\equiv$ classical maxwellians
- Dissipates classical entropy $\int Q(w) \ln w \, dw \leq 0$

Quantum Boltzmann operator

- Requirements:
  - has the same 'shape' as the classical one
  - Preserves mass, momentum and energy locally
  - Kernel $\equiv$ quantum maxwellians
  - Dissipate quantum entropy

$$\int Q(w)\, \mathcal{L}\mathrm{n}\, w \, \frac{dx\, dp}{(2\pi\hbar)^d} \leq 0$$

Quantum Boltzmann operator (cont)

$$Q(w) = \int B(|p - p_1|, \Omega) \\ (A(w)' A(w)'_1 - A(w) A(w)_1) dp_1 \, d\Omega$$

where $A(w)$ is the 'conversion operator':

$$A(w) = \exp \mathcal{L}\mathrm{n}\, w$$

Quantum BGK operator

$$Q(w) = M_w - w$$

where

$$M_w = \mathcal{E}\mathrm{xp}(A + B \cdot p + C|p|^2)$$

s.t.

$$\int (M_w - w)\mu \, dp = 0 \qquad \text{for } \mu = (1, p, |p|^2)$$

7. Quantum Energy-Transport and Drift-Diffusion models

Collaboration w. C. Ringhofer and F. Méhats

Quantum Energy-Transport or Drift-Diffusion

- Rescaled Wigner equation ($\varepsilon \ll 1$)

$$\varepsilon \partial_t w + p \cdot \nabla_x w + \Theta^\hbar[V]w = \varepsilon^{-1} Q(w)$$

- $$Q(w) = M_w - w \qquad M_w = \mathcal{E}\text{xp}(A + C|p|^2)$$

$$\int (M_w - w)\mu \, dp = 0$$

  - $\mu = (1, |p|^2)$ Energy-Transport
  - $\mu = 1; C = -1/2T$ fixed Drift-Diffusion

Quantum Energy-Transport (cont)

- $\varepsilon \longrightarrow 0$ (diffusion approximation)
- Energy transport:

$$\partial_t \int \mathcal{E}\text{xp}(A + C|p|^2) \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp - \int \mathcal{T}^2 \mathcal{E}\text{xp}(A + C|p|^2) \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp = 0$$

with $\mathcal{T} w = (p \cdot \nabla_x + \Theta^\hbar[V])w$

Quantum Drift-Diffusion (cont)

- Drift-Diffusion:

$$\partial_t \int \mathcal{E}\text{xp}(A - |p|^2/2T)\, dp - \int \mathcal{T}^2 \mathcal{E}\text{xp}(A - |p|^2/2T)\, dp = 0$$

- QET and QDD are consistent with quantum entropy dissipation. e.g. ET case:

$$\partial_t S(n, W) \leq 0$$

with $(n, W)^{Tr} = \int \mathcal{E}\text{xp}(A + C|p|^2)(1, |p|^2)^{Tr}\, dp$

$\hbar^2$ expansions of QET and QDD

- $\hbar \to 0$ gives classical ET or DD models (diffusion models)
- $O(\hbar^2)$ corrections to classical DD:

$$\partial_t n - \nabla_x \cdot (T \nabla_x n + n \nabla_x (V + V_B)) = 0$$

V_B = Bohm potential:

$$V_B = -\frac{\hbar^2}{6} \frac{1}{\sqrt{n}} \Delta_x \sqrt{n} = 0$$

$O(\hbar^2)$ corrections to classical DD or ET

- $O(\hbar^2)$ terms in quantum ET $\longrightarrow$ very complex model
- QDD up to $O(\hbar^2)$ terms is consistent with quantum entropy dissipation:

$$\partial_t \tilde{S}(n) \leq 0$$

- QET up to $O(\hbar^2)$ terms is not consistent with quantum entropy dissipation.

8. Summary and conclusion

Summary

- Extension of the Levermore's moment method to the quantum case
  - Take local moments of the density operator eq.
  - Close by a minimizer of the entropy functional
- leads to:
  - Formulation of the entropy minimization problem as a global problem (local in classical mechanics)
  - Non-local closure to the Quantum Hydrodynamics eq.

Summary (cont)

- Quantum collision operators
  - preserve mass, momentum and energy
  - consistent w. quantum entropy decay
  - Boltzmann or BGK type

- Drift-Diffusion or Energy-Transport models
  - through-diffusion approximation of Quantum BGK
  - Justification of Bohm potential in Quantum Drift-Diffusion

- Ref: D., Ringhofer, Mehats.
  See also [Zubarev et al]: NESOM theory

Perspectives

- Verify entropy minimization problem has a solution in a reasonable sense
- Practical computations of model problems with QHD model
- $\hbar^2$ corrections to classical mech.
- Small T asymptotics
- Normal mode analysis of linearized model
- $\ldots$