C. R. Acad. Sci. Paris, Ser. I 335 (2002) 967–972

Physique mathématique/*Mathematical Physics*
(Problèmes mathématiques de la mécanique/*Mathematical Problems in Mechanics*)

A Note on quantum moment hydrodynamics and the entropy principle

Pierre Degond [a], Christian Ringhofer [b]

[a] **MIP (UMR CNRS 5640), Université Paul Sabatier, 118, route de Narbonne, 31062 Toulouse cedex 4, France**

[b] **Department of Mathematics, Arizona State University, Tempe, AZ 85287-1804, USA**

Received 3 June 2002; accepted after revision 16 October 2002

Note presented by Pierre-Louis Lions.

Abstract In this Note, we show how a non-commutative version of the entropy extremalization principle allows one to construct new quantum hydrodynamic models. ***To cite this article: P. Degond, C. Ringhofer, C. R. Acad. Sci. Paris, Ser. I 335 (2002) 967–972.***

Une Note sur l'hydrodynamique des moments quantiques et le principe d'entropie

Résumé Dans cette Note, nous montrons comment une version non-commutative du principe d'extremalisation de l'entropie permet de construire de nouveaux modèles hydrodynamiques quantiques. ***Pour citer cet article : P. Degond, C. Ringhofer, C. R. Acad. Sci. Paris, Ser. I 335 (2002) 967–972.***

Version française abrégée

Dans ce travail, nous proposons une nouvelle approche pour établir des modèles hydrodynamiques quantiques. A partir d'une matrice densité ρ, nous développons un concept de moment local. Etant donné un monôme $p^{\otimes j}$ où p est l'impulsion et j est un multi-indice, on définit le moment m_j de ρ comme l'intégrale (4) où $W[\rho]$ est la transformée de Wigner de ρ (définie par la formule (2)). Lorsque ρ satisfait l'équation de Liouville quantique (1), $W[\rho]$ est solution de l'équation de Wigner (3). On obtient un système d'équations aux moments si, à partir d'un ensemble J de multi-indices j, on multiplie l'équation de Wigner (3) par $p^{\otimes j}$ et on intègre par rapport à p. Bien entendu, de même que dans le cas classique [8], le système aux moments n'est pas fermé, c'est à dire que l'on ne peut écrire la contribution du terme $[H, \rho]$ de l'équation de Liouville quantique comme seule fonction des moments m_j pour $j \in J$. Il convient alors de développer une méthode de fermeture.

Diverses approches de ce problème ont été abordées dans la littérature (voir par exemple [2–7]). Notre approche est inspirée de celle de Levermore [8] pour les modèles classiques (voir également [11]), laquelle utilise un principe d'extrémalisation d'entropie (minimisation ou maximisation selon le signe assigné à l'entropie). Notre approche possède également des similarités avec [9,10,13], mais le concept de moment

E-mail addresses: degond@mip.ups-tlse.fr (P. Degond); ringhofer@asu.edu (C. Ringhofer).

S1631-073X(02)02595-5/FLA

(ou variable localement conservée) dans ces références y est plus vague. Dans le présent travail, nous proposons un cadre précis à ce formalisme. Ce cadre est détaillée de manière plus détaillée dans [1].

Dans le cadre quantique, l'entropie est une observable globale du système (et non locale en chaque point x), définie par $G(\rho) = \mathrm{Tr}(g(\rho))$, où g est une fonction strictement convexe de la variable réelle, $g(\rho)$ est définie à l'aide du calcul fonctionnel et le symbôle Tr désigne la trace d'un opérateur. Dans le cas de l'entropie de Boltzmann, on a classiquement $g(z) = z(\ln z - 1)$. Le principe d'entropie consiste à minimiser $G(\rho)$ sous la contrainte que les moments locaux de ρ sont fixés et donnés par $m = (m_j(x))_{j\in J}$. Dans le contexte quantique, l'expression des contraintes se fait via la transformée de Wigner et conduit au problème (8). Ce problème se résout sous la forme (10), où les multiplicateurs de Lagrange $\mu = (\mu_j(x))_{j\in J}$ sont des fonctions de x. L'expression (10) définit ainsi l'équilibre ρ^m associé au système de moments $m = (m_j(x))_{j\in J}$. Il est à noter que la relation entre les moments m et les multiplicateurs de Lagrange μ est fonctionnelle et non pas locale. A partir de (10), on peut construire un concept d'entropie fluide $S(m) = \mathrm{Tr}(g(\rho^m))$, fonctionnelle strictement convexe de ses arguments m.

Une fois défini le concept d'équilibre (opérateur densité solution du problème de minimisation (8)), il est possible de l'utiliser pour fermer le système aux moments. Pour cela, il suffit de remplacer $[H, \rho]$ par $[H, \rho^m]$ dans les termes correspondants des équations aux moments. Si l'on applique ce principe aux équations de l'hydrodynamique (pour lesquelles l'ensemble des moments est obtenu à partir de $\{p^{\otimes j}, j \in J\} = \{1, p_1, p_2, p_3, |p|^2\}$), on obtient un système d'équations analogue aux équations de l'hydrodynamique classique (12), à ceci près que le tenseurs de pression et le flux de chaleur s'obtiennent par le biais de relations fonctionnelles à partir des trois moments de base (densité, impulsion moyenne et énergie moyenne). En particulier, on ne peut prouver en général que le tenseur des pressions est scalaire et que le flux de chaleur est nul. Cette approche, développée ici de manière purement formelle, pose de nombreuses questions mathématiques qui seront abordées dans des travaux ultérieurs.

---

1. Introduction

This paper is concerned with moment closures of quantum mechanical phase space equations, i.e., the Von Neumann equation for density matrices or, equivalently, the Wigner equation for the Wigner function, leading to so called quantum hydrodynamic systems. The Von Neumann equation for density matrices is given by

$$\mathrm{i}\hbar\partial_t \rho(x, y, t) = [H, \rho], \tag{1}$$

where $\hbar$ is the Planck constant, ρ is the density matrix, H is the Hamiltonian $H = -\frac{\hbar}{2m_*}\Delta + V(x)$ and m_* denotes the effective mass of the particle. The symbol $[\cdot, \cdot]$ denotes the usual commutator. Fluid dynamic approximations to the quantum system are derived by taking local moments of the Von Neumann equation (1). Since taking local moments is a classical concept, this is done most easily by transforming the density matrix into the Wigner function via the Wigner–Weyl transform

$$w(r, p, t) = \hbar^3 W[\rho](r, p, t) = (2\pi)^{-3} \int \rho\left(r - \frac{\hbar}{2}\eta, r + \frac{\hbar}{2}\eta, t\right) \mathrm{e}^{\mathrm{i}\eta\cdot p}\, \mathrm{d}\eta, \tag{2}$$

which yields the Wigner equation

$$\partial_t w + \nabla_r \cdot \left(p\frac{w}{m_*}\right) = \frac{\mathrm{i}}{\hbar} \sum_{\nu=\pm 1} \nu V\left(r + \frac{\nu\hbar}{2\mathrm{i}}\nabla_p\right) w, \tag{3}$$

where the operator on the right-hand side of (3) has to be understood in the sense of pseudo-differential operators [12]. The local moments $m_j(r, t)$ of the Wigner function w w.r.t. the momentum variable p are

given by

$$m_j(r,t) = \int p^{\otimes j} w(r,p,t)\,\mathrm{d}p, \tag{4}$$

for some multi-index j, and fluid equations for the moments m_j are obtained by taking the corresponding moments of the Wigner equation (3). This leads to an infinite system of equations for the moments, which has to be closed, i.e., the higher order moments have to be expressed in terms of the lower order moments by using some ansatz for the Wigner function w or, equivalently, for the density matrix ρ. In the literature, this ansatz is either based on the assumption of a single pure state or, alternatively on some form of random phase approximation [2,7,6] or on some semi-classical approximation of the thermal equilibrium density matrix [3], leading to local quantum corrections of the compressible Euler equation for plasmas in the form of Bohm potentials. A more detailed approximation of the thermal equilibrium density matrix leads to non-local corrections of the Euler equations, where, however, the non-locality enters only through the mean field potential V [4,5]. In the classical case, which is obtained formally by sending $\hbar$ to zero in the Wigner equation, closure is achieved by employing a thermodynamic argument, namely that the phase space density function minimizes an entropy functional locally among all possible phase space densities, which have a certain prescribed set of moments. This leads to a general set of moment closures in the sense of Levermore [8]. In this paper we generalize this concept to the non-commutative algebra of density operators. The result is a set of moment equations which, as in the classical case satisfy a corresponding entropy principle [8]. However, because of the non-local nature of quantum mechanics, the resulting moment equations will have to be non-local as well. A related approach can be found in [9,10,13], where however, the notion of local quantum moment (or locally conserved variable) is more vague. The present approach brings a mathematical framework to these notions. For more detail about the present work, we refer the reader to [1].

2. Entropy principles

In order to translate the concept of entropy closures to the quantum mechanical framework we first consider the classical case. We chose a certain index set J and derive the moment equations for the vector of moments $m(r,t) = \{m_j,\ j \in J\}$ from the Wigner equation (3). Given a convex entropy function $g(w)$ we would then choose the closure function w^m as the phase space density which minimizes the corresponding entropy functional among all densities which possess the given set of moments, i.e.,

$$\int g\big(w^m(r,p,t)\big)\,\mathrm{d}p = \min\left\{ \int g\big(w(r,p,t)\big)\,\mathrm{d}p : \int p^{\otimes j} w(r,p,t)\,\mathrm{d}p = m_j(r,t),\ j \in J \right\} \quad \forall r,t. \tag{5}$$

In the framework of quantum mechanics, taking local moments is replaced by computing the expectation of self adjoint operators, corresponding to observable quantities. Given a self adjoint operator (time dependent) $\mathrm{Op}(a(t))$ with hermitian operator kernel $a(x,y,t)$, the expectation $E[\mathrm{Op}(a)]$ of $\mathrm{Op}(a)$ is computed in terms of the density matrix by the formula

$$E\big[\mathrm{Op}\big(a(t)\big)\big] = \int a(x,y,t)\rho(y,x,t)\,\mathrm{d}x\,\mathrm{d}y = \mathrm{Tr}(a\rho)(t),$$

where the symbol Tr denotes the usual trace of an operator. In the Wigner picture the hermitian operator kernel $a(x,y,t)$ is related to a real-valued function $W[a](r,p,t)$ (the Weyl symbol of $\mathrm{Op}(a)$) via the Weyl quantization formula

$$a(x,y,t) = (2\pi\hbar)^{-3} \int W[a]\left(\frac{x+y}{2}, p, t\right) \exp\left(\mathrm{i}\frac{p}{\hbar}(x-y)\right) \mathrm{d}p.$$

The Weyl quantization formula has the property that the expectation of $\mathrm{Op}(a)$ is computed by integrating $W[a]$ against the Wigner function, i.e., $\mathrm{Tr}(a\rho)(t) = \int W[a](r,p,t)w(r,p,t)\,\mathrm{d}r\,\mathrm{d}p$ holds. Furthermore, self adjoint operators (meaning $a(y,x,t) = a(x,y,t)^*$) correspond to real valued Weyl transforms $W[a]$, and therefore have real expectations. We now generalize the minimization principle (5) by first replacing the local entropy by a global entropy, defining

$$G(\rho) = \mathrm{Tr}\big(g(\rho)\big), \tag{6}$$

where the term $g(\rho)$ denotes the function g evaluated in a functional sense at the operator ρ via the diagonalization of the self adjoint operator ρ. Next, we express the constraints in (5) in a weak form by integrating them against test functions $\lambda_j(r),\ j \in J$:

$$\int \lambda_j(r)\, p^{\otimes j} w(r,p,t)\,\mathrm{d}r\,\mathrm{d}p = \int \lambda_j(r) m_j(r,t)\,\mathrm{d}r \quad \forall t,\ \forall \lambda_j,\ j \in J. \tag{7}$$

Using the properties of the Weyl transform, the quantum equivalent of the minimization problem (5) can be written as

$$G\big(\rho^m\big) = \min\left\{ G(\rho) : \mathrm{Tr}\big(W^{-1}\big[\lambda_j p^{\otimes j}\big]\rho\big) = \int \lambda_j(r) m_j(r,t)\,\mathrm{d}r\ \forall \lambda_j,\ j \in J \right\}. \tag{8}$$

3. Solution of the minimization problem

We now turn to the solution of the minimization problem (8). A necessary condition for the extremality of ρ^m under the constraints given in (8) is that the functional derivative of the functional G vanishes in all directions tangent to the linear manifold given by the constraints. In other words

$$DG\big(\rho^m\big)(\delta\rho) = 0, \quad \text{for all directions } \delta\rho \text{ with } \mathrm{Tr}\big(W^{-1}\big[\lambda_j p^{\otimes j}\big]\delta\rho\big) = 0,\ \forall \lambda,\ j \in J, \tag{9}$$

has to hold, where $DG(\rho^m)(\delta\rho)$ denotes the Gâteaux derivative of G at ρ in the direction $\delta\rho$. To make some practical use of the condition (9) we need the following

THEOREM 1. – *Let the entropy functional $G(\rho)$ be defined as in* (6)*. Then*

$$DG(\rho)(\delta\rho) = \mathrm{Tr}\big(g'(\rho)\delta\rho\big)$$

holds for any self adjoint operators ρ and $\delta\rho$. Furthermore, if g is a strictly convex function on $\mathbb{R}_+$, $G(\rho)$ is a strictly convex functional of the operator ρ.

Using Theorem 1, we now see that $\mathrm{Tr}(g'(\rho)\delta\rho) = 0$ has to hold for all directions $\delta\rho$ satisfying $\mathrm{Tr}(W^{-1}[\lambda_j p^{\otimes j}]\delta\rho) = 0$ for all possible test functions λ_j, $j \in J$. This implies that the matrix $g'(\rho)$ has to be a linear combination of terms of the form $W^{-1}[\lambda_j p^{\otimes j}]$ and we obtain:

COROLLARY 1. – *If the constrained minimization problem* (9) *has a solution it has to satisfy*

$$\rho = (g')^{-1}\left(\sum_{j\in J} W^{-1}\big[\mu_j p^{\otimes j}\big] \right) \tag{10}$$

for some functions $\mu_j(r,t)$, $j \in J$ (the entropy variables), where $(g')^{-1}$ denotes the functional inverse of the real function g' applied to self adjoint operators.

So, the closure of the quantum moment system is given by a density operator ρ^m and its corresponding Wigner function, according to (2), which is of the form (10), where the entropy variables μ_j are related to the moments m_j via

$$\mathrm{Tr}\big(\rho^m W^{-1}\big[\lambda_j p^{\otimes j}\big]\big) = \int \lambda_j(r) m_j(r,t)\,\mathrm{d}r, \quad \forall \lambda_j,\ j \in J. \tag{11}$$

4. The quantum fluid entropy

The closure conditions which arise from the local entropy minimizer derived in the previous section can be quite involved in practice, as will be seen in the next section. However, they do have the advantage that they conserve a convex functional of the moments m_j. If we define the quantum fluid entropy by $S(m) = G(\rho^m)$, it is, as in the classical case, a consequence of the construction, that $S(m)$ will be preserved in time. It remains to show that the functional $S(m)$ is actually a convex functional of the moments m_j which follows from the convexity of the functional G together with the minimization property of ρ^m. We have

THEOREM 2. – *Let the fluid entropy $S(m)$ be defined by $S(m) = G(\rho^m)$, $m = \{m_j,\ j \in J\}$, with ρ^m given by* (11). *Then $S(m)$ is a convex functional of its arguments.*

Proof. – We evaluate the fluid entropy on the straight line between two moment vectors m and m'. By definition we have $S(\tau m + (1-\tau)m') = G(\rho^{\tau m+(1-\tau)m'})$, which, according to (8) satisfies the minimization problem

$$G\big(\rho^{\tau m+(1-\tau)m'}\big) = \min\left\{ G(\rho) : \mathrm{Tr}\big(W^{-1}\big[\lambda_j p^{\otimes j}\big]\rho\big) = \int \lambda_j(r)\big(\tau m_j + (1-\tau)m'_j\big)(r,t)\,\mathrm{d}r\ \forall \lambda_j,\ j \in J \right\}.$$

Now the linear interpolant of the density matrices corresponding to m and m', $\tau\rho^m + (1-\tau)\rho^{m'}$, clearly also satisfies the constraints of the minimization problem. Therefore

$$G\big(\rho^{\tau m+(1-\tau)m'}\big) \leqslant G\big(\tau\rho^m + (1-\tau)\rho^{m'}\big)$$

holds. Using the convexity of the functional G, we conclude that

$$G\big(\rho^{\tau m+(1-\tau)m'}\big) \leqslant \tau G\big(\rho^m\big) + (1-\tau)G\big(\rho^{m'}\big)$$

holds, which gives the convexity of S as a functional of the moments. □

5. The quantum hydrodynamic equations

We now consider one particular realization of the approach outlined in the previous sections, namely the case in which mass momentum and energy are chosen as the moments of the Wigner equation, i.e., $\{p^{\otimes j},\ j \in J\} = \{1, p_1, p_2, p_3, |p|^2\}$ holds. Furthermore we use the fluid dynamical entropy function $g(z) = z(\ln z - 1)$, which implies $g'(z) = \ln z$, $(g')^{-1}(z) = \mathrm{e}^z$. Denoting with $\langle p^{\otimes j}\rangle(r,t) = \int p^{\otimes j} w(r,p,t)\,\mathrm{d}p$ the corresponding moments of the Wigner function we obtain the moment system

$$\begin{aligned} &\text{(a)}\quad m_*\partial_t\langle 1\rangle + \nabla_r\cdot\langle p\rangle = 0, \qquad \text{(b)}\quad m_*\partial_t\langle p\rangle + \nabla_r\cdot\big\langle pp^{\mathrm{T}}\big\rangle = -m_*\langle 1\rangle\nabla_r V, \\ &\text{(c)}\quad m_*\partial_t\big\langle |p|^2\big\rangle + \nabla_r\cdot\big\langle p|p|^2\big\rangle = -2m_*\langle p\rangle\cdot\nabla_r V, \end{aligned} \tag{12}$$

which coincides with the classical hydrodynamic equations. To close the system we have to express the terms $\langle pp^{\mathrm{T}}\rangle$ and $\langle |p|^2 p\rangle$ in terms of the primary variables. According to the previous section, this is done by solving the entropy minimization problem, i.e., by finding entropy variables $\mu_j(r,t)$ such that

$$\operatorname{Tr}\left\{\exp\left(W^{-1}\left[\mu_0+\sum_{j=1}^{3}\mu_j p_j+\mu_4|p|^2\right]\right)W^{-1}\left[\lambda_0+\sum_{j=1}^{3}\lambda_j p_j+\lambda_4|p|^2\right]\right\}$$
$$=\int\left(\lambda_0\langle 1\rangle+\sum_{j=1}^{3}\lambda_j\langle p_j\rangle+\lambda_4\langle|p|^2\rangle\right)\mathrm{d}r \tag{13}$$

holds for all test functions $\lambda_0,\ldots,\lambda_4$. The moment system (12) is then closed by computing the Wigner function corresponding to the minimizer

$$w^m=(2\pi\hbar)^{-3}W\left[\exp\left(W^{-1}\left[\mu_0+\sum_{j=1}^{3}\mu_j p_j+\mu_4|p|^2\right]\right)\right]$$

and from there the moments $\langle pp^{\mathrm{T}}\rangle$ and $\langle|p|^2p\rangle$. So, closing the moment hierarchy with the entropy minimizer involves solving Eq. (13) for a matrix exponential. In practice this procedure will have to be simplified by replacing the exponential function by a suitable rational approximation.

6. Conclusions

We have derived a formalism to close moment hierarchies for quantum mechanical transport equations. This formalism represents the quantum equivalent to classical closures based on locally minimizing (or maximizing if one uses the opposite sign convention) the entropy. It therefore leads to a natural extension of the classical compressible Euler equations, but the same approach can be employed to derive the quantum – equivalent of extended thermodynamics equations [11] or completely general entropy closures [8].

Acknowledgement. The authors acknowledge support from the CNRS-NSF project # 7412 entitled "Modélisation, analyse et simulation des modèles quantiques hybrides et applications aux matériaux semiconducteurs".

References

[1] P. Degond, C. Ringhofer, Quantum moment hydrodynamics and the entropy principle, Manuscript.
[2] D. Ferry, H. Grubin, Modelling of quantum transport in semiconductor devices, Solid State Phys. 49 (1995) 283–448.
[3] C. Gardner, The quantum hydrodynamic model for semiconductor devices, SIAM J. Appl. Math. 54 (1994) 409–427.
[4] C. Gardner, C. Ringhofer, The smooth quantum potential for the hydrodynamic model, Phys. Rev. E 53 (1996) 157–167.
[5] C. Gardner, C. Ringhofer, The Chapman–Enskog expansion and the quantum hydrodynamic model for semiconductor devices, VLSI Design 10 (2000) 415–435.
[6] I. Gasser, P. Markowich, C. Ringhofer, Closure conditions for classical and quantum moment hierarchies in the small temperature limit, Transport Theory Statist. Phys. 25 (1996) 409–423.
[7] H. Grubin, J. Krekovski, Quantum moment balance equations and resonant tunneling structures, Solid State Electron. 32 (1989) 1071–1075.
[8] C.D. Levermore, Moment closure hierarchies for kinetic theories, J. Statist. Phys. 83 (1996) 1021–1065.
[9] R. Luzzi, arXiv: cond-mat/9909160 v2 11 Sep 1999.
[10] V.G. Morozov, G. Röpke, Zubarev's method of a nonequilibrium statistical operator and some challenges in the theory of irreversible processes, Condensed Matter Phys. 1 (1998) 673–686.
[11] I. Muller, T. Ruggeri, Rational Extended Thermodynamics, in: Springer Tracts Nat. Philos., Vol. 37, 2nd edition, Springer, 1998.
[12] M.A. Shubin, Pseudodifferential Operators and Spectral Theory, Springer, 1980.
[13] D.N. Zubarev, V.G. Morozov, G. Röpke, Statistical Mechanics of Nonequilibrium Processes, Vol. 1, Basic Concepts, Kinetic Theory, Akademie-Verlag, Berlin, 1996.