On a New Isothermal Quantum Euler Model: Derivation, Asymptotic Analysis and Simulation

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Abstract. In the first part of this article, we derive a New Isothermal Quantum Euler model. Starting from the quantum Liouville equation, the system of moments is closed by a density operator which minimizes the quantum free energy. Several simplifications of the model are then written for the special case of irrotational flows. The second part of the paper is devoted to a formal analysis of the asymptotic behavior of the quantum Euler system in two situations: at the semiclassical limit and at the zero-temperature limit. The remarkable fact is that in each case we recover a known model: respectively the isothermal Euler system and the Madelung equations. Finally, we give in the third part some preliminary numerical simulations.

1 Introduction

Various works have been devoted in the past decade to the derivation of quantum hydrodynamic models for semiconductors in order to simulate nanoscale devices such as tunneling diodes or lasers. The interest in such models comes from the fact that they are supposed to describe quantum transport in highly collisional situations and to be computationally less expensive than corresponding quantum microscopic models, such as the Schrödinger equation or the Wigner equation.

To design quantum hydrodynamic models with temperature effects, the route which has been usually followed consists in incorporating to classical fluid models some “quantum” correction terms, based on the Bohm potential [5,6,7]. However, such approaches are not obvious to justify from physical principles. Moreover, quantum corrections involving the Bohm potential produce high order terms in these systems and make their resolution difficult, from the mathematical and numerical points of view.

In 2003, Degond and Ringhofer proposed in [3] a different manner to derive quantum hydrodynamic models, by closing the systems of moments thanks to a quantum entropy minimisation principle. This systematic approach, which is an extension of Levermore’s moment method to the framework of quantum mechanics, seems very fruitful, although it is still formal. Following this first

paper, an entropic quantum drift-diffusion model has been derived, analyzed and then discretized numerically in [4]. Numerical comparisons of this model with existing quantum transport models in [2] showed that it is a good candidate model for quantum device simulations in diffusive regimes.

It has been possible to rewrite recently in [1] the isothermal quantum hydrodynamic model in a simpler and differential way. In this article, we remind the methodology used to derive this model.

We also investigate several asymptotic limits for this model: at the semiclassical limit and at the zero-temperature limit. The remarkable fact is that in each case we recover a known model: respectively the isothermal Euler system and the Madelung equations.

Some simplifications of the model for the special case of irrotational flows allow us to present some preliminary numerical results in one dimension.

We finish this introduction by giving some possible applications of the Quantum Euler model. We first have in mind the semiconductor industry where engineers have first introduced Hydrodynamics models with $\hbar^2$ quantum corrections in order to simulate nanoscale devices such as the so-called Resonant Tunneling Diode. The use of these models have permitted to exhibit interesting features of RTD such as negative resistance or hysteresis. The Quantum Euler model could be also used in quantum chemistry, or other areas of physics such as quantum optics, the study of superfluidity, etc...

2 Derivation of the Model

2.1 The Underlying Quantum Microscopic Model

At the microscopic scale, a quantum system evolving in $\mathbb{R}^3$ and subject to a potential $V(x, t)$ can be described by a time-dependent density operator satisfying the quantum Liouville equation:

$$i\hbar\partial_t\varrho = [\mathcal{H}, \rho] + i\hbar\mathcal{Q}(\varrho), \quad (1)$$

where $\hbar$ is the scaled Planck constant and $\mathcal{H}$ is the Hamiltonian:

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

and $\mathcal{Q}(\rho)$ is an unspecified collision operator which describes the interaction of the particles with themselves and with their environment and accounts for dissipation mechanisms. By a density operator, we shall always mean a positive, Hermitian, trace-class operator acting on $L^2(\mathbb{R}^3)$. Let $W[\varrho](x, p)$ denote the Wigner transform of ϱ :

$$W[\varrho](x, p) = \int \underline{\varrho}\left(x - \frac{1}{2}\eta, x + \frac{1}{2}\eta\right) e^{\frac{i\eta \cdot p}{\hbar}} d\eta, \quad (3)$$

where $\underline{\varrho}(x, x')$ is the distribution kernel of ϱ :

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

The inverse Wigner transform (or Weyl quantization) is given by the following formula:

$$W^{-1}[w]\psi(x) = \int w\left(\frac{x+y}{2}, p\right) \psi(y) e^{\frac{ip(x-y)}{\hbar}} \frac{dp dy}{(2\pi\hbar)^3}, \quad (4)$$

and defines $W^{-1}[w]$ as an operator acting on the element ψ of L^2 . The Wigner transform W and its inverse W^{-1} are Isometries between $\mathcal{L}^2$ (the space of operators such that the product $\varrho\varrho^\dagger$ is trace-class, where $\varrho^\dagger$ is the Hermitian conjugate of ϱ) and $L^2(\mathbb{R}^{2d})$:

$$\mathrm{Tr}\{\varrho\sigma^\dagger\} = \int W[\varrho](x, p) \overline{W[\sigma](x, p)} \frac{dx dp}{(2\pi\hbar)^3}. \quad (5)$$

Taking the Wigner transform of (1), we get the following collisional Wigner equation for $w = W[\varrho]$:

$$\partial_t w + p \cdot \nabla_x w + \Theta^\hbar[V]w = Q(w), \quad (6)$$

with

$$\begin{aligned} \Theta^\hbar[V]w = & -\frac{i}{(2\pi)^3\hbar} \int (V(x + \frac{\hbar}{2}\eta) - V(x - \frac{\hbar}{2}\eta)) \times \\ & \times w(x, q) e^{i\eta \cdot (p-q)} dq d\eta. \end{aligned} \quad (7)$$

and $Q(w)$ is the Wigner transform of $\mathcal{Q}(\varrho)$.

2.2 The Moment Method

If we suppose that the collision operator conserves the mass and momentum, integrations with respect to the variable $p \in \mathbb{R}^3$ enable to obtain equations for the first two moments $n(t, x) = \int w(t, x, p) \frac{dp}{(2\pi\hbar)^3}$ (the mass density) and $n(t, x)u(t, x) = \int p w(t, x, p) \frac{dp}{(2\pi\hbar)^3}$ (the current density):

$$\partial_t n + \nabla \cdot nu = 0, \quad (8)$$

$$\partial_t(nu) + \nabla \Pi + n\nabla V = 0. \quad (9)$$

Of course, this system of equations is not closed, since the pressure tensor Π is still expressed in terms of the microscopic Wigner function $w(t, x, p)$:

$$\Pi = \int_{\mathbb{R}^d} p \otimes p w \frac{dp}{(2\pi\hbar)^3}. \quad (10)$$

The quantum Euler model is thus complete only as soon as the closure assumption is made precise. Hence, by analogy with Levermore's methodology [9] and according to [3], we close the system by replacing the expression (10) of Π by another one in terms of n and nu :

$$\Pi = \int_{\mathbb{R}^d} p \otimes p w_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^3}, \quad (11)$$

where $w_{n,nu}^{eq} = W[\varrho_{n,nu}^{eq}]$ is the so-called quantum Maxwellian, depending only on n and nu in a non local (and non explicit) way, as defined in next subsection.

2.3 The Quantum Free Energy Minimization Principle

We intend to describe the effect of the interaction of a quantum system, subject to a potential V , with a thermal bath at temperature T . To this aim, it is convenient to introduce the quantum free energy defined by:

$$G(\varrho) = \text{Tr} \{T(\varrho(\log \varrho - 1)) + \mathcal{H}\varrho\}. \quad (12)$$

where $\mathcal{H} = -\frac{\hbar^2}{2}\Delta + V$ is the Hamiltonian.

The main assumption concerning the interaction between the system and the thermal bath is that the first two moments n and nu are conserved during these interactions. According to this statement, we now claim the quantum free energy minimization principle (the reader can refer to [3] for details). Let the functions n and nu be given. Consider the following constrained minimization problem:

$$\min \left\{ G(\varrho) \text{ such that } \int W[\varrho] \frac{dp}{(2\pi\hbar)^3} = n \text{ and } \int p W[\varrho] \frac{dp}{(2\pi\hbar)^3} = nu \right\}. \quad (13)$$

The solution, if it exists, is called the local equilibrium density operator (or quantum Maxwellian) associated to n and nu . Lagrange multiplier theory for the constrained problem (13) (see [3]) shows that there exist a scalar function A and a vector function B , both real valued and defined on $\mathbb{R}^3$, such that this local equilibrium density operator takes necessarily the form:

$$\varrho_{n,nu}^{eq} = \exp \left(-\frac{1}{T} H(A, B) \right), \quad (14)$$

where $H(A, B)$ is the following modified Hamiltonian:

$$H(A, B) = W^{-1} \left[\frac{1}{2}(p - B)^2 + A \right] = \frac{1}{2} (i\hbar\nabla + B)^2 + A. \quad (15)$$

2.4 The Quantum Euler Model

According to the definition of the quantum Maxwellian (14) and to commutation properties with the Hamiltonian, it is possible to simplify the pressure tensor and to express it with respect to n , nu , A and B (see [1]) and we obtain the following system:

$$\partial_t n + \nabla \cdot nu = 0, \quad (16)$$

$$\partial_t (nu) + \nabla(nu \otimes B) + n(\nabla B) \cdot (u - B) + n\nabla(V - A) = 0, \quad (17)$$

where the extensive quantities n and nu and the associated intensive ones A and B are linked by the following constitutive equations:

$$\begin{aligned} n &= W[\varrho_{n,nu}^{eq}] = \sum_{p \in \mathbb{N}} \exp \left(-\frac{\lambda_p}{T} \right) |\psi_p|^2, \\ nu &= W[p \varrho_{n,nu}^{eq}] = \sum_{p \in \mathbb{N}} \exp \left(-\frac{\lambda_p}{T} \right) \mathcal{Im} (\hbar \nabla \psi_p \overline{\psi_p}), \end{aligned} \quad (18)$$

and where $(\lambda_p, \psi_p)_{p \in \mathbb{N}}$ denotes the complete set of eigenvalues and normalized eigenvectors of the modified Hamiltonian defined by

$$H(A, B) = \frac{1}{2} (i\hbar \nabla + B)^2 + A. \quad (19)$$

2.5 Special Case of Irrotational Flows

We conclude this section by dealing with the special case of irrotational flows. Let n, nu, A, B be given according to the definition of the quantum Maxwellian. Assume moreover that u is an irrotational vector field, *i.e.* that there exists $S(x)$ such that $u = \nabla S$. Then B is defined by

$$B = u = \nabla S \quad (20)$$

In this case, the quantum Euler system (16)–(19) can be rewritten as follows:

$$\partial_t n + \nabla \cdot nu = 0, \quad (21)$$

$$\partial_t(nu) + \nabla(nu \otimes u) + n \nabla(V - A) = 0, \quad (22)$$

where n and A are coupled by the constitutive equation:

$$n = \sum_{p \in \mathbb{N}} \exp\left(-\frac{\lambda_p}{T}\right) |\psi_p|^2, \quad (23)$$

and where $(\lambda_p, \psi_p)_{p \in \mathbb{N}}$ denotes the complete set of eigenvalues and normalized eigenvectors of the modified Hamiltonian defined by

$$H(A, 0) = -\frac{\hbar^2}{2} \Delta + A. \quad (24)$$

As we can see, the system is much simpler in this case since it does not depend on B anymore. The only non-local relation links the intensive variable A to the extensive one n .

3 Formal Asymptotics

We investigate here various asymptotic approximations of the quantum Euler system as dimensionless parameters go to zero. Our aim here is to draw some connections between this model and several other existing models.

3.1 Semiclassical Asymptotics

It is possible to perform an $\hbar$ expansion of the “quantum Maxwellian” $\varrho_{n,nu}^{eq}$. By keeping in this expansion the terms up to the order $\mathcal{O}(\hbar^2)$, one gets formally some approximate constitutive equations linking (n, nu) and (A, B) :

$$A = T \ln n_0 - T \ln n + \frac{\hbar^2}{6} \frac{\Delta \sqrt{n}}{\sqrt{n}} - \frac{\hbar^2}{24} |\omega|^2 + \mathcal{O}(\hbar^4), \quad (25)$$

$$nB = nu + \frac{\hbar^2}{12} \nabla \times (n\omega) + \mathcal{O}(\hbar^4), \quad (26)$$

where we have denoted $\omega = \nabla \times u$ and n_0 is the effective density of state $n_0 = \left(\frac{T}{2\pi\hbar^2}\right)^{3/2}$.

Then, inserting these equations (25), (26) in (16), (17), one gets an approximate quantum Euler model:

$$\partial_t n + \nabla \cdot nu = 0, \quad (27)$$

$$\begin{aligned} \partial_t(nu) + \nabla(nu \otimes u) + T\nabla n + n\nabla V - \frac{\hbar^2}{6} n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) + \\ + \frac{\hbar^2}{12} \omega \times (\nabla \times (n\omega)) + \frac{\hbar^2}{24} n \nabla(|\omega|^2) = \mathcal{O}(\hbar^4). \end{aligned} \quad (28)$$

It is readily seen from (27) and (28) that, as $\hbar \rightarrow 0$, the quantum Euler system converges formally to the isothermal Euler system. Moreover, if we drop the terms $\mathcal{O}(\hbar^4)$ in (27), (28), the obtained model is the so-called quantum hydrodynamic model [7], up to additional terms depending only on $\omega = \nabla \times u$. For irrotational flows, we recover the quantum hydrodynamic model. These observations were already made in [8].

3.2 The Zero Temperature Limit

An opposite limit to the semiclassical asymptotics is the zero-temperature limit. Assume that the solution $(n^T, n^T u^T, A^T, B^T)$ of the quantum Euler system (16)–(19) with temperature T , admits a non trivial limit (n, nu, A, B) as the dimensionless temperature T goes to zero. Then these functions satisfy the Madelung equations:

$$\partial_t n + \nabla \cdot nu = 0, \quad (29)$$

$$\partial_t u + (u \cdot \nabla)u + \nabla V - \frac{\hbar^2}{2} \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0, \quad (30)$$

$$A = \frac{\hbar^2}{2} \frac{\Delta \sqrt{n}}{\sqrt{n}} - C, \quad B = u, \quad (31)$$

where C is a constant and the system is described by a pure-state:

$$\underline{\varrho}(x, x') = \psi(x) \overline{\psi(x')}, \quad (32)$$

with

$$\psi = \sqrt{n} e^{iS/\hbar} \quad \text{and} \quad \nabla S = u.$$

This gives a clear link between the quantum Euler model and the fluid dynamic expression of the Schrödinger equation.

4 Numerical Results

Inspired by the previous work realized for the quantum drift-diffusion model [4,2], we have implemented a 1D numerical scheme for solving the quantum

Fig. 1. Numerical solution of the quantum Euler model with relaxation for $t = 0$, $t = 0.1$ and $t = 1$. Left: density $n(t, x)$ (solid line) and total electrical potential $(V^s + V^{ext})(t, x)$ (dashed line) as functions of the position x . Right: velocity $u(t, x)$ as function of the position x .

Euler system with relaxation coupled to the Poisson equation on the domain $\Omega = [0, 1]$. In 1D, the velocity is of course irrotational so that the quantum Euler model reads under the reduced form (21)-(24), and the Poisson equation is given by:

$$-\alpha^2 \Delta V^s = n, \quad (33)$$

with α the scaled Debye length. We have chosen for the parameters $\hbar^2/2T = 0.1$ and $\alpha^2 = 0.1$. We choose an initial density concentrated on the left of the device and take the initial velocity equal to zero. The external potential V^{ext} is chosen to be a double barrier (in fact, the device here is a simplified Resonant Tunneling Diode without doping) and Figure 1 shows the evolution of the electron density $n(x)$ on the left, and the velocity $u(x)$ on the right for $t = 0$, $t = 0.1$ and $t = 1$. We can see electrons going through the barriers by tunneling effect.

5 Conclusion and Perspectives

In this paper, we have written in a simpler and differential way the isothermal version of the quantum hydrodynamic model derived in [3]. We have then written some formal asymptotics of the model as dimensionless parameters tend to zero. It appears formally that the semiclassical limit of the model is the Classical isothermal Euler system while the zero temperature limit of the model gives the Madelung equations. We have also written several simplifications of the model when the velocity is irrotational which allows us to perform numerical simulations on a simple 1D device. These preliminary numerical simulations seem to indicate that the model gives meaningful results in realistic situations. The study of the numerical scheme together with comparisons with other models will be presented in a future article.

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