

# ISOTHERMAL QUANTUM HYDRODYNAMICS: DERIVATION, ASYMPTOTIC ANALYSIS AND SIMULATION

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**Abstract.** This article is devoted to the reformulation of an isothermal version of the quantum hydrodynamic model (QHD) derived by Degond and Ringhofer in *J. Stat. Phys.* **112** (2003), 587–628 (which will be referred to as the quantum Euler system). We write the model under a simpler (differential) way. The derivation is based on an appropriate use of commutators. Starting from the quantum Liouville equation, the system of moments is closed by a density operator which minimizes the quantum free energy. Some properties of the model are then exhibited and most of them rely on a gauge invariance property of the system. Several simplifications of the model are also 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 three situations: at the semiclassical limit, at the zero-temperature limit and at a diffusive limit. The remarkable fact is that in each case we recover a known model: respectively the isothermal Euler system, the Madelung equations and the entropic quantum drift-diffusion model. Finally, we give in the third part some preliminary numerical simulations.

**Key words.** density matrix, quantum Liouville equation, quantum moment hydrodynamics, local equilibria, entropy minimization, quantum Euler, asymptotic analysis, Madelung equations, entropic quantum drift-diffusion, numerical simulations

**AMS subject classifications.** 82C10, 82C70, 82D37, 81Q05, 81S05, 81S30, 81V70

**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 [1, 6, 23, 24, 25]. It is known since Madelung [22] that the Schrödinger equation can be reformulated in a fluid dynamic way. Indeed, using WKB wave functions  $\psi = \sqrt{n}e^{iS/\hbar}$  enables us to obtain a system on the density  $n(t, x)$  and the velocity  $u = \nabla S(t, x)$  which is formally equivalent to the Schrödinger equation and takes the form of a pressureless Euler system, with an additional term involving the so-called Bohm potential proportional to  $\Delta(\sqrt{n})/\sqrt{n}$  (see (3.6), (3.7)). Unfortunately, this approach is essentially devoted to pure-state quantum mechanics, since it is difficult to adapt it in order to take into account many-body effects and statistical mechanics. In this sense, one can say that the Madelung equations are the zero-temperature quantum hydrodynamic equations.

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 [13, 14, 15, 16, 17, 19]. However, such approaches are not obvious to justify from physical principles. Moreover, quantum corrections involving the Bohm potential produce high order terms in

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these systems and make their resolution difficult, from the mathematical and numerical points of view.

In 2003, Degond and Ringhofer [11] proposed 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 [21] 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 in [10] and after reformulation thanks to elementary algebra in [9], it has been possible to go further in its analysis and to discretize it numerically in [12]. Numerical comparisons of this model with existing quantum transport models in [8] showed that it is a good candidate model for quantum device simulations in diffusive regimes.

Here, we are interested in the hydrodynamic regime with a quantum Euler system, which is nothing but an isothermal version of the quantum hydrodynamic model derived in [11]. Let us shortly present this model (more detail can be found in Section 2, where the derivation of this system is revisited). From the Wigner equation, integrations with respect to the momentum variable  $p \in \mathbb{R}^d$  ( $d$  being the dimension of the momentum space,  $d = 3$  in this paper) enable to obtain equations for the first two moments  $n(t, x)$  (the mass density) and  $n(t, x)u(t, x)$  (the current density), both densities being functions of the space variable  $x \in \mathbb{R}^3$  and the time variable  $t \in \mathbb{R}$ :

$$(1.1) \quad \partial_t n + \operatorname{div}(nu) = 0,$$

$$(1.2) \quad \partial_t(nu) + \operatorname{div}(nu \otimes u + \mathbb{P}) + n\nabla V = 0,$$

where  $V$  denotes an applied potential. Of course, this system of equations is not closed, since the pressure tensor  $\mathbb{P}$  is still expressed in terms of the microscopic Wigner function  $f(t, x, p)$ :

$$(1.3) \quad \mathbb{P} = \int_{\mathbb{R}^d} (p - u)(p - u) f(t, x, p) \frac{dp}{(2\pi\hbar)^d},$$

where  $\hbar$  is the dimensionless Planck constant. The quantum Euler model is thus complete only as soon as the closure assumption is made precise. We close the system by replacing the expression (1.3) of  $\mathbb{P}$  by another one in terms of  $n$  and  $nu$ :

$$(1.4) \quad \mathbb{P} = \int_{\mathbb{R}^d} (p - u)(p - u) f_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^d},$$

where  $f_{n,nu}^{eq}$  is the so-called local equilibrium, depending only on  $n$  and  $nu$  in a non local (and non explicit) way. It is precisely defined in Section 2 as follows:  $f_{n,nu}^{eq} = W[\varrho_{n,nu}^{eq}]$ , where  $W$  is the Wigner transform and  $\varrho_{n,nu}^{eq}$  is the local equilibrium density operator obtained thanks to an entropy minimization principle. The Wigner transform  $W$  and the equilibrium density operator  $\varrho_{n,nu}^{eq}$  will be precisely defined in the next section.

Needless to say, presented in this manner, this quantum Euler model (1.1), (1.2), (1.4) is rather involved and not easy to handle numerically. The aim of this paper is triple. First, as it was done for the entropic quantum drift-diffusion model in [9], we reformulate (in Section 2) this system in a simpler (differential) and more tractable way, and we prove directly a few properties of this model. Note that, to do this, we rederive the model thanks to the entropy minimization principle without using the Wigner formalism, which has in itself an interest since this approach is easily adaptable

to systems set on bounded domains (subject to adequate boundary conditions). We also show some properties of the model, which, for most of them, rely on a gauge invariance property of the system and we write several simplifications of the model for the special case of irrotational flows.

Second, we investigate in Section 3 several asymptotic limits for this model, which enable us to make some links with other models: the isothermal Euler system at the semiclassical limit in section 3.1 (during this asymptotics, we also recover a model obtained by Jüngel and Matthes in [20]), the Madelung equations at the zero-temperature limit (section 3.2) and the entropic quantum drift-diffusion model of [10] at the diffusive limit (section 3.3). Note also that, in this section 3.3, we consider the quantum Euler model with a relaxation term and suggest that this additional term drives the system to global quantum equilibria.

Third, we present as preliminary results in section 4 some numerical simulations to illustrate the model on a simple device. A future article will be devoted to the study of the numerical scheme employed here and comparisons with other models will be performed.

The main results of this paper are thus Theorem 2.5, reformulating the quantum Euler system, Proposition 2.8, dealing with the special case of irrotational flows, and Theorems 3.3, 3.5, 3.8 and 3.9 dealing with its asymptotic approximations. We wish to precise that the arguments presented in this article are formal. A precise mathematical framework in which this analysis could be made rigorous is still to be found.

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. One nanoscale device of interest is the so-called Resonant Tunneling Diode [4]. The use of these models have permitted to exhibit interesting features of RTD such as negative resistance or hysteresis [5, 18]. The Quantum Euler model could be also used in quantum chemistry [3], or other areas of physics such as quantum optics, the study of superfluidity, etc...

**2. Derivation of the model and main properties.** In this section, we recall how the strategy of Degond and Ringhofer [11] enables to derive a closed system of moment equations with a constant temperature. The key ingredient is a free energy (instead of an entropy) minimization principle. It gives rise to the notion of local equilibrium microscopic state which is chosen in order to close the system of moments. This argument is shortly presented in subsection 2.2 and in the beginning of subsection 2.3. The quantum Euler system is then rewritten under a simplified form in Theorem 2.5, which gathers the main new result of this section.

**2.1. Notations.** By a density operator, we shall always mean a positive, Hermitian, trace-class operator acting on  $L^2(\mathbb{R}^3)$ . Let us define the first moments of a density operator  $\varrho$ , *i.e.* the mass density  $n$  and the current density  $nu$ , by duality, considering scalar test functions  $\phi$  and vector ones  $\Phi$ . We set

$$(2.1) \quad \forall \phi \in C_0^\infty(\mathbb{R}^3) \quad \int n\phi \, dx = \text{Tr}\{\varrho\phi\},$$

$$(2.2) \quad \forall \Phi \in C_0^\infty(\mathbb{R}^3)^3 \quad \int nu \cdot \Phi \, dx = \text{Tr} \left\{ \varrho W^{-1} [p \cdot \Phi] \right\} = -i\hbar \text{Tr} \left\{ \varrho \left( \Phi \cdot \nabla + \frac{1}{2}(\text{div}\Phi) \right) \right\}$$

(in the right-hand sides,  $\phi$ ,  $\Phi$  and  $\text{div}\Phi$  are the multiplication operators). Note that an immediate consequence of (2.1) and (2.2) is the following property which will be useful later:

$$(2.3) \quad \forall \Phi \quad -\frac{i}{\hbar} \text{Tr}\{\varrho(\Phi \cdot \nabla)\} = \int nu \cdot \Phi \, dx + \frac{i\hbar}{2} \int n \, \text{div}\Phi \, dx.$$

In (2.2),  $W^{-1}$  denote the inverse Wigner transform (or Weyl quantization). For the sake of completeness, let us recall the definition of the Wigner transform and the inverse Wigner transform. The Wigner transform maps operators on  $L^2(\mathbb{R}^3)$  to symbols, *i.e.*  $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$  functions of the classical position and momentum variables  $(x, p) \in \mathbb{R}^3 \times \mathbb{R}^3$ . More precisely, one defines the integral kernel of the operator  $\varrho$  to be the distribution  $\underline{\varrho}(x, x')$  such that  $\varrho$  operates on any function  $\psi(x) \in L^2(\mathbb{R}^3)$  as follows:

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

Then, the Wigner transform  $W[\varrho](x, p)$  is defined by:

$$(2.4) \quad W[\varrho](x, p) = \int \underline{\varrho}\left(x - \frac{1}{2}\eta, x + \frac{1}{2}\eta\right) e^{\frac{i\eta \cdot p}{\hbar}} d\eta.$$

The Wigner transform can be inverted and its inverse is defined for any function  $f(x, p)$  as the operator acting on  $\psi(x) \in L^2(\mathbb{R}^3)$  as:

$$(2.5) \quad W^{-1}[f]\psi(x) = (2\pi\hbar)^{-3} \int f\left(\frac{x+y}{2}, p\right) \psi(y) e^{\frac{ip(x-y)}{\hbar}} dp dy.$$

We end this section by expressing a few commutator identities that are used in the sequel of this article. Let  $\phi(x)$ ,  $\psi(x)$ ,  $\Phi(x)$ ,  $\Psi(x)$  be test functions (the capital letters are used for vector functions while the lower case letters are used for scalar ones). Then, the following equalities hold:

$$(2.6) \quad [\phi, \psi] = 0,$$

$$(2.7) \quad [\phi, \Psi \cdot \nabla] = -\Psi \cdot \nabla \phi,$$

$$(2.8) \quad [\Phi \cdot \nabla, \Psi \cdot \nabla] = ((\Phi \cdot \nabla)\Psi - (\Psi \cdot \nabla)\Phi) \cdot \nabla,$$

$$(2.9) \quad [\phi, \Delta] = -\Delta\phi - 2\nabla\phi \cdot \nabla.$$

We also recall the cyclicity of the trace, where  $a, b, c$  are three operators:

$$\text{Tr}\{[a, b]c\} = \text{Tr}\{[c, a]b\} = \text{Tr}\{[b, c]a\}.$$

**2.2. Local equilibria via entropy minimization.** Let  $s$  be a strictly convex continuously differentiable function on  $\mathbb{R}^+$ . We define the quantum entropy by:

$$(2.10) \quad S(\varrho) = \text{Tr}\{s(\varrho)\}.$$

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:

$$(2.11) \quad G(\varrho) = TS(\varrho) + E(\varrho) = \text{Tr}\{Ts(\varrho) + \mathcal{H}\varrho\}.$$

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 in the following definition (the reader can refer to [11] for details):

DEFINITION 2.1. *Let the functions  $n$  and  $nu$  be given. Consider the following constrained minimization problem:*

$$(2.12) \quad \min \{G(\varrho) \text{ such that } \varrho \text{ is a density operator satisfying (2.1) and (2.2)}\}.$$

The solution, if it exists, is called the local equilibrium density operator associated to  $n$  and  $nu$ . Lagrange multiplier theory for the constrained problem (2.12) (see [11]) 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:

$$(2.13) \quad \varrho_{n,nu}^{eq} = (s')^{-1} \left( -\frac{1}{T} H(A, B) \right),$$

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

$$(2.14) \quad H(A, B) = W^{-1} \left[ \frac{1}{2}(p - B)^2 + A \right] = \frac{1}{2} (i\hbar\nabla + B)^2 + A.$$

This definition is obviously incomplete if no assumption is made on  $n$  and  $nu$ . In fact, this result has to be understood only at a formal level. Several crucial questions remain open: in which functional spaces  $n$  and  $nu$  have to be chosen, in which spaces  $A$  and  $B$  have to be sought, or the question of existence and uniqueness of  $A$  and  $B$ . Throughout this paper, we shall postpone this delicate question of realizability of moments, assuming that, as soon as the minimization problem (2.12) has to be solved,  $n$  and  $nu$  are such that the associate functions  $A$  and  $B$  are uniquely defined. In fact, since we are dealing with trace-class operators, the mass and current densities  $n$  and  $nu$  vanish at the infinity and it seems reasonable to assume that the modified Hamiltonian  $H(A, B)$  has always a compact resolvent and thus a discrete spectrum  $(\lambda_p(A, B))_{p \in \mathbb{N}}$  and a complete set of (normalized) eigenfunctions denoted by  $(\psi_p(A, B))_{p \in \mathbb{N}}$ . According to these assumptions, one can rewrite the mass density and the current density associated to  $\varrho_{n,nu}^{eq}$  in terms of the eigen-elements of  $H(A, B)$ :

$$(2.15) \quad n(A, B) = \sum_{p \in \mathbb{N}} (s')^{-1} \left( -\frac{\lambda_p(A, B)}{T} \right) |\psi_p(A, B)|^2,$$

$$(2.16) \quad (nu)(A, B) = \sum_{p \in \mathbb{N}} (s')^{-1} \left( -\frac{\lambda_p(A, B)}{T} \right) \mathcal{I}m \left( \hbar\nabla\psi_p(A, B) \overline{\psi_p(A, B)} \right).$$

REMARK 2.2 (Towards a numerical method to compute  $A$  and  $B$ ). *The constitutive equations (2.15)–(2.16) provide no explicit relation between the extensive quantities  $(n, nu)$  and the associate intensive quantities  $(A, B)$ . Nevertheless, we can provide a practical method to compute  $A^0$  and  $B^0$  associated to given  $n^0$  and  $n^0 u^0$ .*

*Consider the change of variable  $\tilde{A} = -A - B^2/2$  and  $\tilde{B} = B$  so that the following Hamiltonian  $\tilde{H}(\tilde{A}, \tilde{B})$  is now linear in  $(\tilde{A}, \tilde{B})$ :*

$$\tilde{H}(\tilde{A}, \tilde{B}) = H(A, B) = -\frac{\hbar^2}{2}\Delta + i\hbar\tilde{B} \cdot \nabla + i\hbar/2 \operatorname{div}\tilde{B} - \tilde{A},$$

and consider the following functional:

$$(2.17) \quad \tilde{\Sigma}(\tilde{A}, \tilde{B}) = T \text{Tr} \left\{ s^* \left( -\frac{1}{T} \tilde{H}(\tilde{A}, \tilde{B}) \right) \right\} := \Sigma(A, B),$$

where  $s^*$  is the convex conjugate function of  $s$  defined such that  $(s^*)' = (s')^{-1}$  (note that this functional, called the Massieu-Planck potential, is in fact the Legendre dual of the quantum free energy [2]). The Gâteaux derivative of  $\tilde{\Sigma}$  can be computed (using a formula which can be found for instance in [11] or [10]) and gives:

$$(2.18) \quad \frac{\delta \tilde{\Sigma}}{\delta \tilde{A}} = n(A, B) \quad ; \quad \frac{\delta \tilde{\Sigma}}{\delta \tilde{B}} = (nu)(A, B).$$

Let define now the following functional:

$$(2.19) \quad J(\tilde{A}, \tilde{B}) = \Sigma(A, B) - \int n^0 \tilde{A} dx - \int n^0 u^0 \cdot \tilde{B} dx,$$

so that the Gâteaux derivative of  $J$  is given by:

$$(2.20) \quad \frac{\delta J}{\delta \tilde{A}} = n(A, B) - n^0 \quad ; \quad \frac{\delta J}{\delta \tilde{B}} = (nu)(A, B) - n^0 u^0.$$

We deduce that if  $J$  admits a critical point  $(\tilde{A}^0, \tilde{B}^0)$ , then the functions  $A^0 = -\tilde{A}^0 - (\tilde{B}^0)^2/2$  and  $B^0 = \tilde{B}^0$  are associated to  $n^0$  and  $n^0 u^0$  according to Definition 2.1. Note that the functional  $J$  is strictly convex due to the fact that  $s^*$  is strictly convex, that  $\tilde{H}(\tilde{A}, \tilde{B})$  is linear in  $(\tilde{A}, \tilde{B})$ , and that the two integrals are linear in  $(\tilde{A}, \tilde{B})$ . This remark allows us to elaborate a numerical method based on a minimization algorithm to compute  $A^0$  and  $B^0$  corresponding to given  $n^0$  and  $n^0 u^0$ .

LEMMA 2.3 (Gauge invariance). *Let  $S(x)$  be a smooth function. Then, we have:*

$$(2.21) \quad \exp \left( \frac{iS}{\hbar} \right) H(A, B) \exp \left( -\frac{iS}{\hbar} \right) = H(A, B + \nabla S).$$

As a consequence we have the following identities:

$$(2.22) \quad n(A, B + \nabla S) = n(A, B) \quad ; \quad (nu)(A, B + \nabla S) = (nu)(A, B) + n(A, B) \nabla S,$$

which relates the density and velocity for two values of  $B$  differing by a gradient.

*Proof.* To prove identity (2.21), we remark that

$$\exp \left( \frac{iS}{\hbar} \right) (i\hbar \nabla + B) \exp \left( -\frac{iS}{\hbar} \right) = i\hbar \nabla + B + \nabla S.$$

Hence

$$\exp \left( \frac{iS}{\hbar} \right) \left( \frac{1}{2} (i\hbar \nabla + B)^2 + A \right) \exp \left( -\frac{iS}{\hbar} \right) = \frac{1}{2} (i\hbar \nabla + B + \nabla S)^2 + A,$$

which is (2.21).

As a consequence, the eigenvalues of  $H(A, B)$  and  $H(A, B + \nabla S)$  are the same. Also, if two operators are conjugate, any function of these two operators are also conjugate by the same conjugation operator. This implies that:

$$(2.23) \quad \exp \left( \frac{iS}{\hbar} \right) s^* \left( -\frac{1}{T} H(A, B) \right) \exp \left( -\frac{iS}{\hbar} \right) = s^* \left( -\frac{1}{T} H(A, B + \nabla S) \right),$$

where  $s^*$  is the convex conjugate function of  $s$  defined such that  $(s^*)' = (s')^{-1}$ . Therefore, the eigenvalues of  $s^* \left(-\frac{1}{T}H(A, B)\right)$  and  $s^* \left(-\frac{1}{T}H(A, B + \nabla S)\right)$  are the same and we have the following equality for the functional  $\Sigma$  defined in (2.17):

$$(2.24) \quad \Sigma(A, B + \nabla S) = \Sigma(A, B),$$

and in particular, we have:

$$(2.25) \quad \frac{\delta \Sigma}{\delta A}(A, B + \nabla S) = \frac{\delta \Sigma}{\delta A}(A, B) \quad ; \quad \frac{\delta \Sigma}{\delta B}(A, B + \nabla S) = \frac{\delta \Sigma}{\delta B}(A, B).$$

Using the formula of the Gâteaux derivative of  $\Sigma$  given in (2.18) and the chain rule leads to:

$$(2.26) \quad \frac{\delta \Sigma}{\delta A} = -n \quad ; \quad \frac{\delta \Sigma}{\delta B} = nu - nB,$$

where  $n$  and  $nu$  shortly denote here  $n(A, B)$  and  $(nu)(A, B)$ , so that identities (2.22) stem directly from (2.25) and (2.26).  $\square$

We end this subsection by giving a lemma which will be needed in the proof of the main result (Theorem 2.5) of the next subsection. This lemma expresses the very strong result that  $u$  and  $B$  are not equal but differ by a vector field which is a curl divided by the density.

LEMMA 2.4. *Let  $n, nu, A, B$  be given according to Definition 2.1. Then we have*

$$(2.27) \quad \operatorname{div}(nu) = \operatorname{div}(nB).$$

*Proof.* The proof of this lemma is a direct consequence of (2.24) and (2.26). We have indeed for any test function  $S(x)$ :

$$\begin{aligned} \lim_{t \rightarrow 0} (t^{-1}(\Sigma(A, B + t\nabla S) - \Sigma(A, B))) &= 0 \\ &= \int \frac{\delta \Sigma}{\delta B} \cdot \nabla S \, dx \\ &= \int (nu - nB) \cdot \nabla S \, dx, \end{aligned}$$

meaning that  $\operatorname{div}(nu - nB) = 0$  almost everywhere.  $\square$

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

$$(2.28) \quad i\hbar \partial_t \varrho = [\mathcal{H}, \varrho] + i\hbar \mathcal{Q}(\varrho),$$

where  $[\mathcal{H}, \varrho] = \mathcal{H}\varrho - \varrho\mathcal{H}$  is the commutator of the Hamiltonian  $\mathcal{H} = -\frac{\hbar^2}{2}\Delta + V$  with the density operator  $\varrho$  and  $\hbar$  is the scaled Planck constant. In the right-hand side of this equation, we have introduced a collision term  $\mathcal{Q}(\varrho)$ . The precise form of this operator will not play an important role in this article. The key property that we request is that it drives the system to the local equilibria defined in the previous section. This is a consequence of the two following assumptions:

- (i) mass and momentum are conserved during collision, *i.e.* for any density operator  $\varrho$  we have

$$(2.29) \quad \forall \varphi, \Phi \quad \text{Tr}\{\mathcal{Q}(\varrho)\varphi\} = 0 \quad \text{and} \quad \text{Tr}\left\{\mathcal{Q}(\varrho)\left(\Phi \cdot \nabla + \frac{1}{2}(\text{div}\Phi)\right)\right\} = 0.$$

- (ii) the quantum free energy is dissipated, except for the density operator in the kernel of  $\mathcal{Q}$ , which is explicitly described as follows:

$$(2.30) \quad \mathcal{Q}(\varrho) = 0 \text{ iff } \exists(A, B) \text{ such that } \varrho = (s')^{-1} \left( -\frac{1}{T} \left( \frac{1}{2}(i\hbar\nabla + B)^2 + A \right) \right).$$

For  $\varrho(t)$  solving (2.28), let us write the equations satisfied by the corresponding moments  $n$  and  $nu$ . To this aim, we first take the trace of the Liouville equation (2.28) against a test function  $\phi$ . Using (2.29), the cyclicity of the trace and the commutator equalities (2.6)–(2.9), we get

$$\begin{aligned} \int \phi \partial_t n \, dx &= \text{Tr}\{\phi \partial_t \varrho\} = -\frac{i}{\hbar} \text{Tr}\{\phi [\mathcal{H}, \varrho]\} = -\frac{i}{\hbar} \text{Tr}\left\{\phi \left[-\frac{\hbar^2}{2}\Delta + V, \varrho\right]\right\} \\ &= -\frac{i}{\hbar} \text{Tr}\left\{\left[\phi, -\frac{\hbar^2}{2}\Delta + V\right] \varrho\right\} = -\frac{i\hbar}{2} \text{Tr}\{(\Delta\phi + 2\nabla\phi \cdot \nabla)\varrho\}. \end{aligned}$$

Now we can use property (2.3) to write:

$$\int \phi \partial_t n \, dx = -\frac{i\hbar}{2} \int n \Delta\phi \, dx + \int nu \cdot \nabla\phi \, dx + \frac{i\hbar}{2} \int n \text{div}(\nabla\phi) \, dx = \int nu \cdot \nabla\phi \, dx.$$

This is the weak formulation of the equation of conservation of mass:

$$(2.31) \quad \partial_t n + \text{div}(nu) = 0.$$

In order to obtain the second moment equation, we compose the collisional Liouville equation (2.28) with the operator  $W^{-1}(p \cdot \Phi) = -i\hbar(\Phi \cdot \nabla + \frac{1}{2}(\text{div}\Phi))$ . Thanks to (2.29), we obtain

$$(2.32) \quad \forall \Phi \quad \int \Phi \cdot \partial_t(nu) \, dx = -\text{Tr}\left\{[\mathcal{H}, \varrho]\left(\Phi \cdot \nabla + \frac{1}{2}(\text{div}\Phi)\right)\right\}.$$

It is readily seen that, with no further assumption, the right-hand side of (2.32) cannot be expressed in terms of  $n$ ,  $nu$  and the test function  $\Phi$  only. We just recover here the fact that the system (2.31), (2.32) – which is equivalent to (1.1), (1.2), (1.3) after Wigner transformation – is not closed.

Hence, by analogy with Levermore's methodology [21] and according to [11], we modify this system by replacing  $\varrho$  in the right-hand side of (2.32) by the Ansatz  $\varrho_{n,nu}^{eq}$ , which plays the role of a Maxwellian here. This Ansatz corresponds to the modeling assumptions (i) and (ii) made on  $\mathcal{Q}$ , and represents the most likely quantum microscopic state which possesses the moments  $n$  and  $nu$ , according to the statistics that has been chosen, *i.e.* the function  $s$ . We point out the fact that  $\varrho_{n,nu}^{eq}$  depends locally in time but globally in space on  $n$  and  $nu$ . Let us now gather the equations forming the quantum Euler model. This system is composed of the two equations governing the time evolution of  $n$  and  $nu$ , (2.31) and

$$(2.33) \quad \forall \Phi \quad \int \Phi \cdot \partial_t(nu) \, dx = -\text{Tr}\left\{[\mathcal{H}, \varrho_{n,nu}^{eq}]\left(\Phi \cdot \nabla + \frac{1}{2}(\text{div}\Phi)\right)\right\},$$



coupled to the constitutive equations

$$(2.34) \quad \varrho_{n,nu}^{eq} = (s')^{-1} \left( -\frac{1}{T} H(A, B) \right) = (s')^{-1} \left( -\frac{1}{2T} (i\hbar\nabla + B)^2 - \frac{A}{T} \right).$$

$$(2.35) \quad \forall \phi \quad \text{Tr}\{\varrho_{n,nu}^{eq} \phi\} = \int n \phi \, dx,$$

$$(2.36) \quad \forall \Phi \quad -i\hbar \text{Tr} \left\{ \varrho_{n,nu}^{eq} \left( \Phi \cdot \nabla + \frac{1}{2}(\text{div}\Phi) \right) \right\} = \int nu \cdot \Phi \, dx.$$

The main result of this section is the following:

**THEOREM 2.5.** *The above described quantum Euler system (2.31), (2.32), (2.34), (2.35), (2.36) is formally equivalent to the following system of equations:*

$$(2.37) \quad \partial_t n + \text{div}(nu) = 0,$$

$$(2.38) \quad \partial_t(nu) + \text{div}(nu \otimes B) + n(\nabla B) \cdot (u - B) + n\nabla(V - A) = 0,$$

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

$$(2.39) \quad n = \sum_{p \in \mathbb{N}} (s')^{-1} \left( -\frac{\lambda_p}{T} \right) |\psi_p|^2, \quad nu = \sum_{p \in \mathbb{N}} (s')^{-1} \left( -\frac{\lambda_p}{T} \right) \mathcal{I}m(\hbar\nabla\psi_p \bar{\psi}_p),$$

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

$$(2.40) \quad H(A, B) = \frac{1}{2} (i\hbar\nabla + B)^2 + A.$$

Moreover, the time evolution of the macroscopic quantum free energy

$$(2.41) \quad \mathcal{G}(t) = \text{Tr} \left\{ Ts(\varrho_{n,nu}^{eq}) + \left( -\frac{\hbar^2}{2} \Delta + V \right) \varrho_{n,nu}^{eq} \right\}, \quad \text{where } \varrho_{n,nu}^{eq} \text{ is defined by (2.34),}$$

is simply given by:

$$(2.42) \quad \frac{d}{dt} \mathcal{G}(t) = \int n \partial_t V \, dx.$$

*Proof.* Let us first prove (2.38). Noticing that the Hamiltonian  $\mathcal{H}$  can be rewritten as:

$$\mathcal{H} = H(A, B) - i\hbar B \cdot \nabla - \frac{i\hbar}{2}(\text{div}B) + V - A - \frac{1}{2}B^2$$

and that  $H(A, B)$  commutes with  $\varrho_{n,nu}^{eq}$  (denoted shortly  $\varrho$  in the sequel of the proof), we obtain from (2.33):

$$\begin{aligned} \int \Phi \cdot \partial_t(nu) \, dx &= \text{Tr} \left\{ (\Phi \cdot \nabla) \left[ i\hbar B \cdot \nabla + \frac{i\hbar}{2}(\text{div}B) - V + A + \frac{1}{2}B^2, \varrho \right] \right\} \\ &\quad + \frac{1}{2} \text{Tr} \left\{ (\text{div}\Phi) \left[ i\hbar B \cdot \nabla + \frac{i\hbar}{2}(\text{div}B) - V + A + \frac{1}{2}B^2, \varrho \right] \right\} \\ &= (I) + (II) + (III) + (IV) \end{aligned}$$

with

$$(I) = i\hbar \text{Tr}\{[\Phi \cdot \nabla, B \cdot \nabla]\varrho\}, \quad (II) = -\frac{i\hbar}{2} \text{Tr}\{[\text{div}B, \Phi \cdot \nabla]\varrho\}$$

$$(III) = \text{Tr}\left\{\left[V - A - \frac{1}{2}B^2, \Phi \cdot \nabla\right]\varrho\right\}, \quad (IV) = \frac{i\hbar}{2} \text{Tr}\{[\text{div}\Phi, B \cdot \nabla]\varrho\}.$$

It remains to make these four terms more explicit. The use of the commutator equality (2.8) and the use of property (2.3) give:

$$(I) = i\hbar \text{Tr}\{\varrho((\Phi \cdot \nabla)B - (B \cdot \nabla)\Phi) \cdot \nabla\}$$

$$= - \int nu \cdot ((\Phi \cdot \nabla)B - (B \cdot \nabla)\Phi) dx - \frac{i\hbar}{2} \int n \text{div}((\Phi \cdot \nabla)B - (B \cdot \nabla)\Phi) dx.$$

A direct computation of the commutators (using (2.7)) in (II), (III) and (IV) gives then:

$$(II) = \frac{i\hbar}{2} \text{Tr}\{((\Phi \cdot \nabla)\text{div}B)\varrho\} = \frac{i\hbar}{2} \int n(\Phi \cdot \nabla)\text{div}B dx,$$

$$(III) = -\text{Tr}\left\{\left(\Phi \cdot \nabla\left(V - A - \frac{1}{2}B^2\right)\right)\varrho\right\} = - \int n(\Phi \cdot \nabla)\left(V - A - \frac{1}{2}B^2\right) dx,$$

$$(IV) = -\frac{i\hbar}{2} \text{Tr}\{B \cdot \nabla \text{div}\Phi\varrho\} = -\frac{i\hbar}{2} \int nB \cdot \nabla \text{div}\Phi dx.$$

It is easy to check that the sum of (II), (IV) and of the imaginary part of (I) vanishes, it remains:

$$\int \Phi \cdot \partial_t(nu) dx = - \int nu \cdot ((\Phi \cdot \nabla)B - (B \cdot \nabla)\Phi) dx - \int n\Phi \cdot \nabla\left(V - A - \frac{1}{2}B^2\right) dx,$$

which after an integration by parts gives the second equation of the quantum Euler system (2.38). This last equation reads componentwise (we use Einstein's convention for the implicit summation on  $j$ ):

$$\partial_t(nu_i) + \partial_j(nu_i B_j) + n(u_j - B_j)\partial_i B_j + n\partial_i(V - A) = 0.$$

Finally, let us show the equation (2.42) for the quantum free energy. To do so, we recall that the derivative of the quantum entropy  $S(\varrho) = \text{Tr}\{s(\varrho)\}$  with respect to  $\varrho$  is (see [11]):

$$dS(\varrho) \cdot \delta\varrho = \text{Tr}\{s'(\varrho)\delta\varrho\}.$$

The derivative of the quantum free energy  $G$  defined by (2.11) with respect to  $\varrho$  is then:

$$(2.43) \quad dG(\varrho) \cdot \delta\varrho = \text{Tr}\{(Ts'(\varrho) + \mathcal{H})\delta\varrho\}.$$

It allows to compute the derivative of  $\mathcal{G} = G(\varrho(t))$  with respect to  $t$  which is given by:

$$(2.44) \quad \frac{d}{dt}\mathcal{G} = \text{Tr}\{(Ts'(\varrho) + \mathcal{H})\partial_t\varrho\} + \int n \partial_t V dx,$$

where we remarked that  $\text{Tr} \{(\partial_t V)\varrho\} = \int n \partial_t V dx$ . Then, we use the Ansatz

$$\varrho = (s')^{-1} \left( -\frac{1}{T} H(A, B) \right),$$

which gives

$$\begin{aligned} \text{Tr} \{(Ts'(\varrho) + \mathcal{H})\partial_t \varrho\} &= \text{Tr} \{(-H(A, B) + \mathcal{H})\partial_t \varrho\} \\ &= \text{Tr} \left\{ \left( -ihB \cdot \nabla - \frac{i\hbar}{2} (\text{div}(B)) + V - A - \frac{1}{2} B^2 \right) \partial_t \varrho \right\} \\ &= \int \left( B \cdot \partial_t(nu) + \partial_t n \left( V - A - \frac{1}{2} B^2 \right) \right) dx. \end{aligned}$$

Using the two equations of the quantum Euler system (2.37), (2.38), we obtain:

$$\begin{aligned} \text{Tr} \{(Ts'(\varrho) + \mathcal{H})\partial_t \varrho\} &= \int B \cdot (-\text{div}(nu \otimes B) - n(\nabla B) \cdot (u - B) - n\nabla(V - A)) dx \\ &\quad - \int \text{div}(nu) \left( V - A - \frac{1}{2} B^2 \right) dx. \end{aligned}$$

The first line in the right-hand side can be simplified after integrations by parts:

$$\begin{aligned} &\int (-B_i \partial_j (nu_i B_j) - nB_i (u_j - B_j) (\partial_i B_j) - nB_i \partial_i (V - A)) dx \\ &= \int \text{div}(nB) \left( V - A - \frac{1}{2} B^2 \right) dx. \end{aligned}$$

So we finally obtain:

$$\text{Tr} \{(Ts'(\varrho) + \mathcal{H})\partial_t \varrho\} = - \int \text{div}(nu - nB) \left( V - A - \frac{1}{2} B^2 \right) dx.$$

This last term vanishes using Lemma 2.4, and finally (2.44) yields (2.42).  $\square$

Let us now write several equivalent formulations of the second equation (2.38), that will be useful further. Direct calculations using (2.37), (2.38) and (2.27) lead to the following equations, which can replace (2.38) in the whole quantum Euler system:

$$(2.45) \quad \partial_t(nu) + \text{div}(nu \otimes u) + n(\nabla \times u) \times (B - u) + n\nabla \left( V - A - \frac{1}{2} |B - u|^2 \right) = 0,$$

$$(2.46) \quad \text{or} \quad \partial_t u + (B \cdot \nabla)u + (\nabla B) \cdot (u - B) + \nabla(V - A) = 0,$$

$$(2.47) \quad \text{or again,} \quad \partial_t u + (\nabla \times u) \times B + \nabla \left( u \cdot B - \frac{1}{2} B^2 + V - A \right) = 0.$$

REMARK 2.6. If we choose for the entropy function  $s(\varrho)$  the Boltzmann entropy:

$$(2.48) \quad s(\varrho) = \varrho(\log \varrho - 1),$$

then the corresponding solution of the quantum free energy minimization problem (2.13) is the equilibrium introduced in [11] as a “quantum equilibrium” and referred as “quantum Maxwellian” in [9]:

$$(2.49) \quad \varrho^m = \exp \left( -\frac{1}{T} H(A, B) \right).$$

The macroscopic quantum free energy corresponding to the Boltzmann entropy reads (dropping the constant term  $\int nTdx$ ):

$$(2.50) \quad \text{Tr} \left\{ T_s(\varrho^m) + \left( -\frac{\hbar^2}{2} \Delta + V \right) \varrho^m \right\} = \int \left( nu \cdot B + n \left( V - A - \frac{1}{2} B^2 \right) \right) dx.$$

We have shown in Theorem 2.5 that if the electric potential  $V$  is independent of time, then this quantum free energy is conserved. In the case where the electrical potential is the sum of an external potential  $V^{ext}$  independent of time and a selfconsistent potential  $V^s$  linked to the charge density by the Poisson equation:

$$(2.51) \quad -\alpha^2 \Delta V^s = n,$$

with  $\alpha$  the scaled Debye length, then the conserved quantity reads:

$$\int \left( nu \cdot B + n \left( V^{ext} - A - \frac{1}{2} B^2 \right) \right) dx + \frac{\alpha^2}{2} \int |\nabla V^s|^2 dx.$$

**2.4. Special case of irrotational flows.** We conclude this section by dealing with the special case of irrotational flows. Before giving the main proposition which is Proposition 2.8, we state the following lemma:

LEMMA 2.7. *Let  $n, nu, A, B$  be given according to Definition 2.1. 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*

$$(2.52) \quad B = u = \nabla S$$

and we have

$$(2.53) \quad \varrho_{n,nu}^{eq} = e^{iS/\hbar} \varrho_{n,0}^{eq} e^{-iS/\hbar},$$

where the two equilibrium density operators  $\varrho_{n,nu}^{eq}$  and  $\varrho_{n,0}^{eq}$  are given according to Definition 2.1. If we note  $n(A, B)$  the density associated to  $A$  and  $B$ , we have moreover:

$$(2.54) \quad n(A, B) = n(A, 0).$$

*Proof.* See Appendix A.  $\square$

PROPOSITION 2.8. *Let  $n, nu$  satisfy the quantum Euler system (2.37)–(2.40). Then  $\omega = \nabla \times u$  satisfies formally the following transport equation:*

$$(2.55) \quad \partial_t \omega + \nabla \times (\omega \times B) = 0.$$

Moreover, assume that at  $t = 0$  the velocity is irrotational, i.e. that we have

$$(2.56) \quad \omega(t = 0) = \nabla \times u(t = 0) = 0,$$

and that the solution of (2.37)–(2.40) is smooth. Then for all time we have  $\omega = \nabla \times u = 0$ . In this case, the quantum Euler system (2.37)–(2.40) can be rewritten as follows:

$$(2.57) \quad \partial_t n + \text{div}(nu) = 0,$$

$$(2.58) \quad \partial_t(nu) + \text{div}(nu \otimes u) + n \nabla(V - A) = 0,$$

where  $n$  and  $A$  are coupled by the constitutive equation:

$$(2.59) \quad n = \sum_{p \in \mathbb{N}} (s')^{-1} \left( -\frac{\lambda_p}{T} \right) |\psi_p|^2,$$

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

$$(2.60) \quad H(A, 0) = -\frac{\hbar^2}{2} \Delta + A.$$

*Proof.* The equation for the curl (2.55) is a direct consequence of (2.47). Now, multiply (2.55) by  $\omega$  and integrate on  $\mathbb{R}^3$ . Straightforward calculations lead to the following equation, governing the evolution of the  $L^2$  norm of  $\omega$ :

$$(2.61) \quad \frac{d}{dt} \int |\omega|^2 dx = - \int (\operatorname{div} B) |\omega|^2 dx + \int (\nabla B) : (\omega \otimes \omega) dx.$$

Hence, applying a Cauchy-Schwarz inequality, we get

$$\frac{d}{dt} \int |\omega|^2 dx \leq C \|\nabla B\|_{L^\infty} \int |\omega|^2 dx,$$

which gives  $\omega \equiv 0$  as soon as  $\omega(t=0) = 0$ , by the Gronwall lemma. Then  $\nabla \times u = 0$  implies that the results of Lemma 2.7 hold true for all time. Hence  $u = B$ , together with (2.38) (or (2.45)), gives (2.58), while  $n(A, B) = n(A, 0)$  is equivalent to (2.59), (2.60), and the proof is complete.  $\square$

**REMARK 2.9.** *In this situation of irrotational flows, the “quantum part” of the model is simpler than in the general case of Theorem 2.5, since the underlying minimization problem is (A.1) given in Appendix, with only the constraint of the first moment  $n$ , instead of (2.12). In the specific case of dimension 1, the flow is obviously generically irrotational, so the quantum Euler system always appears under the reduced form (2.57)–(2.60).*

**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. All the proofs given in this section use formal arguments.

**3.1. Semiclassical asymptotics.** If we choose for the entropy function  $s$  the Boltzmann entropy (2.48), then an  $\hbar$  expansion of the “quantum Maxwellian”  $\varrho_{n,nu}^{eq}$  can be performed. 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  $(A, B)$ :

**LEMMA 3.1 (formal).** *Let  $n, nu, A, B$  be smooth functions linked according to Definition 2.1 with the entropy function  $s$  being the Boltzmann entropy (2.48). As the dimensionless Planck constant  $\hbar$  goes to 0, the quantities  $A$  and  $B$  admit the following asymptotic expansions:*

$$(3.1) \quad A = T \ln n_0 - T \ln n + \frac{\hbar^2}{6} \frac{\Delta \sqrt{n}}{\sqrt{n}} - \frac{\hbar^2}{24} |\omega|^2 + \mathcal{O}(\hbar^4),$$

$$(3.2) \quad nB = nu + \frac{\hbar^2}{12} \nabla \times (n\omega) + \mathcal{O}(\hbar^4),$$

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

*Proof.* See Appendix B.  $\square$

REMARK 3.2. In reduced dimension  $d = 2$  or  $d = 1$ , the expression of the effective density of state  $n_0$  has to be replaced by  $n_0 = \left(\frac{T}{2\pi\hbar^2}\right)^{d/2}$ . Then, inserting these equations (3.1), (3.2) in (2.37), (2.45), one gets an approximate quantum Euler model.

THEOREM 3.3 (Semiclassical formal limit). *Let the entropy function  $s$  be the Boltzmann entropy (2.48). Then, as the dimensionless Planck constant  $\hbar$  goes to 0, the quantum Euler system admits the following asymptotic expansion:*

$$(3.3) \quad \partial_t n + \operatorname{div}(nu) = 0,$$

$$(3.4) \quad \begin{aligned} \partial_t(nu) + \operatorname{div}(nu \otimes u) + T\nabla n + n\nabla V - \frac{\hbar^2}{6} n\nabla \left( \frac{\Delta\sqrt{n}}{\sqrt{n}} \right) + \\ + \frac{\hbar^2}{12} \omega \times (\nabla \times (n\omega)) + \frac{\hbar^2}{24} n\nabla(|\omega|^2) = \mathcal{O}(\hbar^4), \end{aligned}$$

where we have denoted  $\omega = \nabla \times u$ .

It is readily seen from (3.3) and (3.4) 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 (3.3), (3.4), the obtained model is the so-called quantum hydrodynamic model [19], 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 [20]. We point out the fact that, if the obtained equations (3.3), (3.4) are rigorously equivalent to the ones obtained by Jüngel and Matthes, *i.e.* (5) and (6) of [20], the method to get them is simpler here and does not require an expansion of the second order moments (1.4) of the Wigner function.

**3.2. The zero temperature limit.** An opposite limit to the semiclassical asymptotics is the zero-temperature limit. Before investigating the formal limit of (2.37)–(2.40) as  $T \rightarrow 0$ , let us claim that, when  $B$  is a gradient, the functions  $A$  and  $B$  can always be explicitly deduced from the ground state of the modified Hamiltonian. Indeed, straightforward (formal) calculations lead to the following lemma:

LEMMA 3.4. *Let  $A$  and  $B$  be given real functions, respectively scalar and vector valued, and assume the existence of a scalar potential  $\varphi(x)$  such that  $B = \nabla\varphi$ . Consider the operator*

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

and assume that the problem of minimization of the energy

$$\min_{|\psi|_{L^2}=1} \int (H(A, B)\psi) \bar{\psi} dx = \min_{|\psi|_{L^2}=1} \int \left( \frac{1}{2} |i\hbar\nabla\psi + B\psi|^2 + A|\psi|^2 \right) dx$$

is attained on the ground state  $\psi_0 = \sqrt{n_0} e^{iS_0/\hbar}$ . Then we have the identities

$$(3.5) \quad A = \frac{\hbar^2}{2} \frac{\Delta\sqrt{n_0}}{\sqrt{n_0}} - C, \quad B = \nabla S_0,$$

where  $C$  is a constant (the Lagrange multiplier corresponding to the constraint).

*Proof.* We remark that the energy of a wavefunction  $\psi = \sqrt{n} e^{iS/\hbar}$  can be rewritten in terms of  $n$  and  $S$ :

$$\int \left( \frac{1}{2} |i\hbar \nabla \psi + B\psi|^2 + A |\psi|^2 \right) dx = \int \left( \frac{1}{2} n |\nabla(S - \varphi)|^2 + \frac{\hbar^2}{2} |\nabla \sqrt{n}|^2 + A n \right) dx.$$

By writing that  $(n_0, S_0)$  minimizes this expression and that  $\sqrt{n_0}$  solves the corresponding Euler-Lagrange equation, we get

$$A = \frac{\hbar^2}{2} \frac{\Delta \sqrt{n_0}}{\sqrt{n_0}} - C, \quad \nabla(S_0 - \varphi) = 0$$

where  $C$  is the Lagrange multiplier corresponding to the equality constraint ( $|\psi|_{L^2} = 1$ ) and the proof is complete. Note that, since  $\psi_0$  is a ground state, by Krein-Rutman's theorem we have  $n_0 > 0$  everywhere, hence we do not have to introduce a Lagrange multiplier for the positivity constraint.  $\square$

We can now claim the following formal result:

**THEOREM 3.5** (Zero temperature formal limit). *Assume that the entropy function  $s$  is such that  $\lim_{+\infty}(s')^{-1} = +\infty$  and  $\lim_{-\infty}(s')^{-1} = 0$ . Assume that the solution  $(n^T, n^T u^T, A^T, B^T)$  of the quantum Euler system (2.37)–(2.40) 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:*

$$(3.6) \quad \partial_t n + \operatorname{div}(nu) = 0,$$

$$(3.7) \quad \partial_t u + (u \cdot \nabla)u + \nabla V - \frac{\hbar^2}{2} \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0,$$

$$(3.8) \quad A = \frac{\hbar^2}{2} \frac{\Delta \sqrt{n}}{\sqrt{n}} - C, \quad B = u,$$

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

$$(3.9) \quad \underline{\varrho}(x, x') = \psi(x) \overline{\psi(x')},$$

with

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

*Proof.* By assumption, if  $A^T$  and  $B^T$  admit a smooth limit, the modified Hamiltonian defined by (2.40) does not behave singularly and its eigenvalues  $(\lambda_p^T)_{p \in \mathbb{N}}$  and eigenfunctions  $(\psi_p^T)_{p \in \mathbb{N}}$  also converge to some limits as  $T \rightarrow 0$ . The limit ground state  $\psi_0$  is not degenerate. Therefore, it follows from the assumption on  $s$  and from (2.39) that  $\lambda_0^T$  must converge to 0, otherwise  $n$  would be either infinite, or zero (note that the limit density  $n$  is assumed to be non trivial). Due to the gap between the first eigenvalue  $\lambda_0$  and the other ones  $\lambda_p, p > 0$  (this gap is supposed to be a consequence of the fact that  $A^T$  and  $B^T$  admit a smooth limit, as well as the non degeneracy of the ground state – this is a strong assumption), we have  $-\lambda_p/T \rightarrow -\infty$  and one can deduce from (2.39) that the occupation factor of the state  $\psi_p$  converges to 0 if  $p > 0$ . Consequently, the limit density operator is that of a pure-state, given by (3.9).

Remark that one must have the following asymptotic behavior for the ground state energy  $\lambda_0^T$ :

$$\lambda_0^T \sim -Ts' \left( \int n \, dx \right) \quad \text{as } T \rightarrow 0.$$

Since at the limit the dynamic is given by the ground state, the corresponding velocity is a gradient:  $u = \nabla S$ , thus by Lemma 2.7, we have  $B = \nabla S$ . Next, by applying Lemma 3.4 we obtain (3.8). Finally, by inserting these relations in (2.46), we obtain the Madelung equation (3.7).  $\square$

REMARK 3.6. *The Boltzmann distribution  $(s')^{-1} = \exp$  corresponding to the entropy  $s(\varrho) = \varrho \ln(\varrho) - \varrho$  satisfies the assumption of Theorem 3.5. But the Fermi-Dirac distribution does not. In this case, since the occupation factors converge to 1 as  $-\lambda_p/T$  tends to  $-\infty$ , one can see that the limit density operator may not be a pure-state but rather a finite rank projector*

$$\underline{\varrho}(x, x') = \sum_{k=1}^K \psi_k(x) \overline{\psi_k(x')},$$

which unfortunately does not enable to obtain the simplified constitutive equations (3.8).

**3.3. System with relaxation, long-time behavior, diffusive limit.** In this section, we come back to the derivation of the quantum Euler system and modify the microscopic description. We rewrite the quantum Liouville equation (2.28), assuming now that the collision operator is composed of two parts, in order to take into account the coexistence of different types of collisions:

$$(3.10) \quad \partial_t \varrho = -\frac{i}{\hbar} [\mathcal{H}, \varrho] + \frac{1}{\varepsilon} \mathcal{Q}_0(\varrho) + \frac{1}{\tau} \mathcal{Q}_1(\varrho).$$

The mean collision times  $\varepsilon$  and  $\tau$  are both assumed to be small, but such that  $\varepsilon \ll \tau$ , which means a hierarchy between the collision phenomena. The predominant collision operator  $\mathcal{Q}_0$  is supposed to be similar as in section 2.3, satisfying the same two assumptions (i) and (ii), whereas the new operator  $\mathcal{Q}_1$  models collisions which do not preserve momentum. To make the analysis simpler, we choose for  $\mathcal{Q}_1$  the quantum BGK operator that was introduced in [10]. It reads

$$\mathcal{Q}_1[\varrho] = \varrho_{n,0}^{eq} - \varrho,$$

since one can see (e.g. in the proof of Lemma 2.7 in the Appendix A) that the equilibrium function with vanishing current  $\varrho_{n,0}^{eq}$  realizes the following minimization problem with mass density constraint:

$$(3.11) \quad \min \left\{ G(\varrho) \text{ such that } \forall \phi \quad \text{Tr}\{\varrho \phi\} = \int n \phi \, dx \right\}.$$

In [10], the diffusive limit of (3.10) without the  $\mathcal{Q}_0$  operator was performed and lead to a model called the entropic quantum drift-diffusion (eQDD) system (the study of this model was continued in [9, 12, 8]). In this section, we follow a different route, that will finally lead to the same model. We perform formally successively two limits. First, in the first Theorem 3.8 of this section, we make  $\varepsilon$  tend to 0 in (3.10), which



corresponds to the *hydrodynamic* asymptotics. The so-obtained model is the quantum Euler system with a relaxation term induced by the new collision operator  $\mathcal{Q}_1$ . We show that this model is entropic and that its equilibria are the usual *global* quantum equilibria. Then, we let  $\tau$  tend to 0, which corresponds to the *diffusive* asymptotics. During this step performed in Theorem 3.9, we recover the eQDD model. In order to prepare this second step, it is now more convenient to rescale the time variable in (3.10), setting  $t = t'/\tau$  (and then dropping the prime):

$$(3.12) \quad \tau \partial_t \varrho = -\frac{i}{\hbar} [\mathcal{H}, \varrho] + \frac{1}{\varepsilon} \mathcal{Q}_0(\varrho) + \frac{1}{\tau} \mathcal{Q}_1(\varrho).$$

Before giving the main result of this section (Theorem 3.8), let us give a lemma which will be needed in the proof:

LEMMA 3.7. *Let  $n, nu, A, B$  be given according to Definition 2.1. Then we have*

$$(3.13) \quad \int nu \cdot B \, dx \geq 0,$$

and this integral vanishes if and only if  $u = B = 0$ .

*Proof.* See Appendix C.  $\square$

THEOREM 3.8 (Hydrodynamic formal limit). *Consider a solution of the quantum Liouville equation (3.12), denoted by  $\varrho^{\varepsilon, \tau}$ . As  $\varepsilon$  goes to 0, this density operator converges formally to the solution*

$$\varrho^\tau = (s')^{-1} \left( -\frac{1}{T} H(A, B) \right)$$

of the following quantum Euler system with relaxation:

$$(3.14) \quad \tau \partial_t n + \operatorname{div}(nu) = 0,$$

$$(3.15) \quad \tau \partial_t (nu) + \operatorname{div}(nu \otimes B) + n(\nabla B) \cdot (u - B) + n \nabla(V - A) = -\frac{1}{\tau} nu,$$

$$(3.16) \quad n = \sum_{p \in \mathbb{N}} (s')^{-1} \left( -\frac{\lambda_p}{T} \right) |\psi_p|^2, \quad nu = \sum_{p \in \mathbb{N}} (s')^{-1} \left( -\frac{\lambda_p}{T} \right) \operatorname{Im}(\hbar \nabla \psi_p \overline{\psi_p}),$$

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

$$(3.17) \quad H(A, B) = \frac{1}{2} (i\hbar \nabla + B)^2 + A.$$

Assume now that the potential  $V$  is independent of time. Then the above model is entropic, i.e. dissipates the quantum free energy defined by (2.11):

$$(3.18) \quad \frac{d}{dt} G(\varrho^\tau(t)) = -\frac{1}{\tau^2} \int nu \cdot B \, dx \leq 0.$$

This suggests that its solution  $\varrho^\tau$  converges at  $t \rightarrow +\infty$  to the global quantum equilibria

$$\varrho_\infty = (s')^{-1} \left( -\frac{1}{T} \left( -\frac{\hbar^2}{2} \Delta + V - \mu_F \right) \right),$$

where the Fermi level  $\mu_F$  is a constant.

*Proof.* The first part of this theorem is mainly an adaptation of the proof of Theorem 2.5. Indeed, by multiplying (3.12) by  $\varepsilon$  and using  $\varepsilon \ll \tau$ , we obtain formally that

$$\mathcal{Q}_0(\varrho^{\varepsilon,\tau}) \rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0.$$

Hence, if  $\varrho^{\varepsilon,\tau}$  converges to a certain  $\varrho^\tau$ , then we have  $\mathcal{Q}_0(\varrho^\tau) = 0$ , and the assumption (2.30) made on  $\mathcal{Q}_0$  implies the existence of  $A$  and  $B$  such that

$$\varrho^\tau = (s')^{-1} \left( -\frac{1}{T} ((i\hbar\nabla + B)^2 + A) \right),$$

or, in other terms, that  $\varrho^\tau = \varrho_{n,nu}^{eq}$ . To conclude, it remains to write the equations satisfied by the two first moments of  $\varrho^{\varepsilon,\tau}$  and to close this system thanks to this expression. The same calculations as for Theorem 2.5 lead to (3.14) and (3.15), taking care of the right-hand sides, which are obtained from  $\mathcal{Q}_1$  by remarking that

$$\forall \phi \quad \text{Tr} \{ \mathcal{Q}_1(\varrho)\phi \} = \text{Tr} \{ (\varrho_{n,0}^{eq} - \varrho)\phi \} = 0,$$

$$\begin{aligned} \forall \Phi \quad -i\hbar \text{Tr} \{ \mathcal{Q}_1(\varrho) (\Phi \cdot \nabla + \frac{1}{2}(\text{div}\Phi)) \} &= -i\hbar \text{Tr} \{ (\varrho_{n,0}^{eq} - \varrho) (\Phi \cdot \nabla + \frac{1}{2}(\text{div}\Phi)) \} \\ &= - \int nu \cdot \Phi \, dx, \end{aligned}$$

thanks to the definition of  $\varrho_{n,0}^{eq}$  and by (2.2).

Moreover, by adapting the proof of (2.42) in Theorem 2.5, one gets easily the equation (3.18) for the evolution of the free energy. Note that the nonpositivity of this term is not trivial and comes from the inequality (3.13) of Lemma 3.7. Finally, by simply considering (3.18), we claim that, as  $t \rightarrow +\infty$ , the relaxation term created by  $\mathcal{Q}_1$  drives the system to equilibria such that  $\int nu \cdot B \, dx = 0$ . Hence, by the second part of Lemma 3.7, these equilibria must be such that  $nu = 0$ . Then, from (3.15), we get  $n\nabla(V - A) = 0$  and  $A = V - \mu_F$ .  $\square$

**THEOREM 3.9** (Diffusive formal limit). *Consider a solution  $\varrho^\tau$  of the quantum Euler model with relaxation (3.14)–(3.17). Then, as  $\tau$  goes to zero,  $\varrho^\tau$  converges formally to the solution*

$$(3.19) \quad \varrho = (s')^{-1} \left( -\frac{1}{T} H(A, 0) \right)$$

of the quantum drift-diffusion system:

$$(3.20) \quad \partial_t n - \text{div}(n\nabla(V - A)) = 0,$$

$$(3.21) \quad n = \sum_{p \in \mathbb{N}} (s')^{-1} \left( -\frac{\lambda_p}{T} \right) |\psi_p|^2,$$

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

$$(3.22) \quad H(A, 0) = -\frac{\hbar^2}{2} \Delta + A.$$

*Proof.* Multiplying (3.15) by  $\tau$ , one can see that  $nu = \mathcal{O}(\tau)$ . Hence, from Lemma 2.7, and assuming that the relation between  $(n, nu)$  and  $(A, B)$  is smooth, we infer  $B = \mathcal{O}(\tau)$ . As a first consequence, we obtain that  $\varrho^\tau$  converges to a certain  $\varrho$  given by (3.19). Secondly, by using again (3.15) and identifying the terms of order zero in  $\tau$ , we get

$$(3.23) \quad -\frac{1}{\tau}nu = n\nabla(V - A) + \mathcal{O}(\tau).$$

By inserting this identity into (3.14) and passing to the limit  $\tau \rightarrow 0$ , we deduce (3.20).  $\square$

**REMARK 3.10.** *The eQDD model, obtained as the limit of an entropic model, is also entropic. Let us give the expression of the corresponding entropy flux. At the diffusive limit  $\tau \rightarrow 0$ , (3.23) shows that  $u/\tau$  converges to the gradient function  $-\nabla(V - A)$ , so Lemma 2.7 gives that, asymptotically, we have  $B = u$ . Therefore, one deduces from (3.18) that the solution of the eQDD system (3.20)–(3.22) satisfies*

$$\frac{d}{dt}G(\varrho(t)) = - \int n|\nabla(V - A)|^2 dx \leq 0.$$

*We recover here an identity that was shown in [10] and, again, the fact that the equilibria are such that  $V - A$  is constant.*

**4. Numerical results.** We have implemented a 1D numerical scheme for solving the quantum Euler system with relaxation coupled to the Poisson equation on the domain  $\Omega = [0, 1]$  in the case where the entropy  $s$  is the Boltzmann entropy. As noticed in Remark 2.9, the quantum Euler system in one dimension takes the reduced form (2.57)–(2.60). Let  $\Delta t > 0$  be the time step and  $\Delta x = 1/N$  ( $N \in \mathbb{N}$ ) the space grid size. The grid is composed of the points  $x_i = i\Delta x$  for  $0 \leq i \leq N + 1$  and we note the unknowns at time  $t = k\Delta t$  as vectors  $n^k = (n_i^k)_{0 \leq i \leq N+1}$ ,  $u^k = (u_i^k)_{0 \leq i \leq N+1}$ ,  $A^k = (A_i^k)_{0 \leq i \leq N+1}$ ,  $V^{s,k} = (V_i^{s,k})_{0 \leq i \leq N+1}$ . For the sake of readability, we also introduce as intermediate unknowns the density and velocity fluxes noted  $j^{k+1/2} = (j_i^{k+1/2})_{0 \leq i \leq N+1}$  and  $\varphi^{k+1/2} = (\varphi_i^{k+1/2})_{0 \leq i \leq N+1}$ . The discretized model reads for  $1 \leq i \leq N$ :

$$(4.1) \quad \tau \frac{n_i^{k+1} - n_i^k}{\Delta t} + \frac{j_i^{k+1/2} - j_{i-1}^{k+1/2}}{\Delta x} = 0,$$

$$(4.2) \quad \tau \frac{u_i^{k+1} - u_i^k}{\Delta t} + \frac{\varphi_{i+1}^{k+1/2} - \varphi_i^{k+1/2}}{\Delta x} = -\frac{u_i^{k+1}}{\tau},$$

$$(4.3) \quad j_i^{k+1/2} = n_i^k u_i^{k+1}$$

$$(4.4) \quad \varphi_i^{k+1/2} = \frac{(u_i^k)^2}{2} + V_i^{ext} + V_i^{s,k+1} - A_i^{k+1}$$

$$(4.5) \quad -\alpha^2 \frac{V_{i+1}^{s,k+1} - 2V_i^{s,k+1} + V_{i-1}^{s,k+1}}{\Delta x^2} = n_i^{k+1}$$

$$(4.6) \quad n_i^{k+1} = \sum_{1 \leq p \leq N} e^{-\frac{\lambda_p(A^{k+1})}{T}} |\psi_{p,i}(A^{k+1})|^2,$$

where  $(\lambda_p(A^{k+1}), \psi_p(A^{k+1}))_{1 \leq p \leq N}$  denotes the eigenvalues and normalized eigenvectors of the  $N \times N$  matrix discretizing the modified Hamiltonian (We put Dirichlet

conditions on the eigenfunctions):

$$H(A^{k+1}, 0) = -\frac{\hbar^2}{2\Delta x^2} \begin{pmatrix} -2 & 1 & 0 & \dots \\ 1 & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & 1 \\ \vdots & 0 & 1 & -2 \end{pmatrix} + \text{Diag}((A_i^{k+1})_{1 \leq i \leq N}).$$

We use for boundary conditions a zero-flux condition which reads:

$$\varphi_{N+1/2}^{k+1/2} = \varphi_N^{k+1/2} \quad ; \quad \varphi_{0}^{k+1/2} = \varphi_1^{k+1/2}.$$

This scheme draws its inspiration from the ones used for the entropic Quantum Drift-Diffusion model in [12, 8]. In order to solve this scheme, we first eliminate  $u_i^{k+1}$ ,  $j_i^{k+1/2}$  and  $\varphi_i^{k+1/2}$  in equation (4.1) using equations (4.2), (4.3) and (4.4). Then we write  $n_i^{k+1}$  as a function of  $A^{k+1}$  in (4.1) using equation (4.6). We obtain a non linear (and not local) system with unknowns  $A_i^{k+1}$  and  $V_i^{s,k+1}$ . It can be shown that this system has a good variational formulation (inspired by Remark 2.2) and can be solved using the Newton algorithm. A future article will be devoted to the study of this scheme. A validation of the model is also needed and comparisons will be performed with other existing models stated above (the quantum hydrodynamics model, the Schrödinger model and the entropic quantum drift-diffusion model).

The values of the parameters are given in Table 4.1. We choose for initial density  $n^0(x)$  a density concentrated on the left of the device and for initial velocity  $u^0(x) = 0$ . 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 Figures 4.2, 4.3 show the evolution of the electron density  $n^k$  on the left, and the velocity  $u^k$  on the right for  $k = 1, 4, 20, 100$  and  $200$ . We can see electrons going through the barriers by tunneling effect. At time step  $k = 200$  the system seems to achieve an equilibrium. This is confirmed by next Figure 4.1 which shows that the free energy  $G(k) = \int \left( n^k \left( V^{ext} - A^k + \left( \frac{u^k}{2} \right)^k \right) \right) dx + \frac{\alpha^2}{2} \int |\nabla V^{s,k}|^2 dx$  does not evolve any more. We can see on this last graph that, as expected, the free energy is a decreasing function of time.

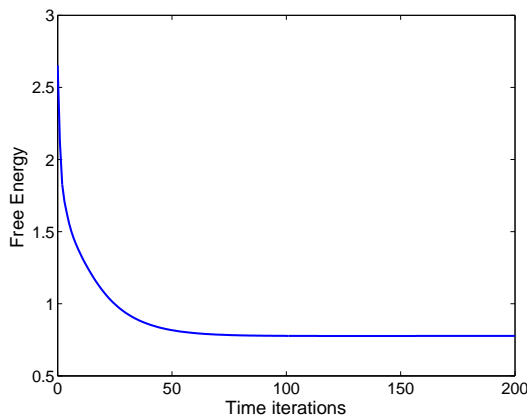


FIGURE 4.1. Evolution of the free energy  $G^k$  as a function of the time iteration  $k$ .

$\Delta x$	$\Delta t$	$\hbar^2/2T$	$\alpha^2$	$\tau$
0.01	0.005	0.02	0.1	0.1

TABLE 4.1

Values of the parameters for the numerical simulation.

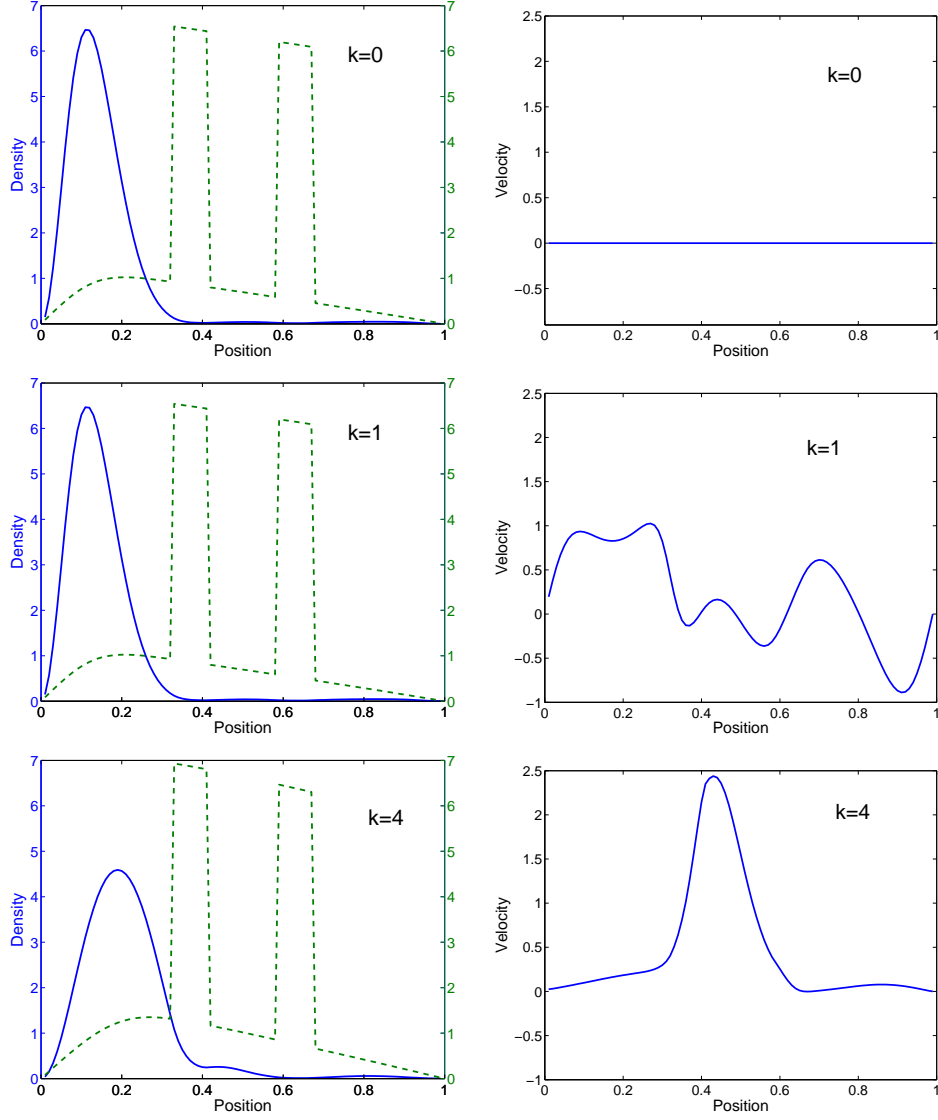


FIGURE 4.2. Numerical solution of the quantum Euler model with relaxation:  $k = 0$  corresponds to the initial data while  $k = 1$  and  $k = 4$  correspond to the solution of the scheme after 1 and 4 iterations. Left: density  $n^k(x)$  (solid line) and total electrical potential  $(V^{s,k} + V^{ext})(x)$  (dashed line) as functions of the position  $x$ . Right: velocity  $u^k(x)$  as function of the position  $x$ .

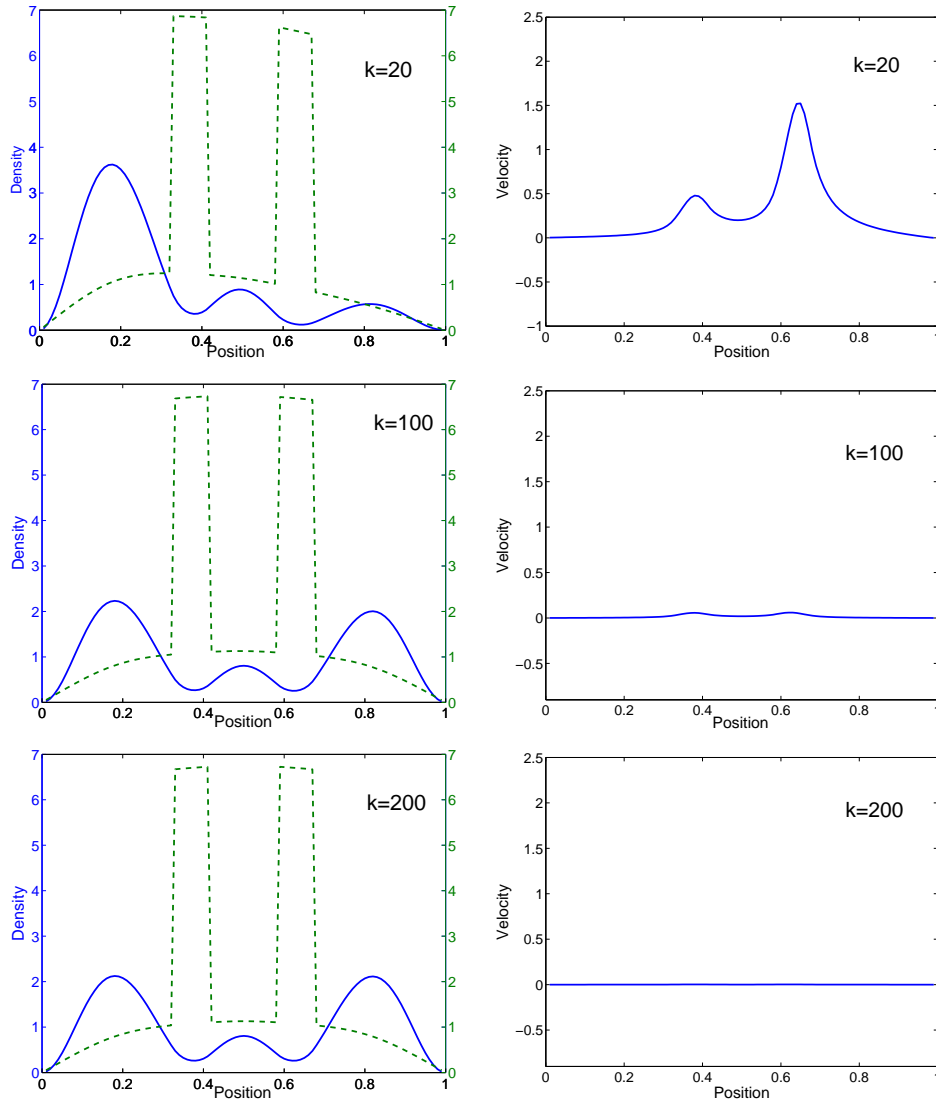


FIGURE 4.3. Numerical solution of the quantum Euler model with relaxation after 20, 100 and 200 iterations. Left: density  $n^k(x)$  (solid line) and total electrical potential  $(V^{s,k} + V^{ext})(x)$  (dashed line) as functions of the position  $x$ . Right: velocity  $u^k(x)$  as function of the position  $x$ .

**5. Conclusion and perspectives.** In this paper, we have rewritten in a simpler and differential way the isothermal version of the quantum hydrodynamic model derived in [11]. A remarkable gauge invariance property for this system has been exhibited. As a by-product, a constraint between the velocity  $u$  and its adjoint variable  $B$  has been discovered. Several equivalent formulations of the model are possible. 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, finally, the diffusive limit permits to show a link with the recently derived entropic Quantum Drift-Diffusion model. We have also written several simplifications of the model when the velocity is irrotational, since in this case,  $u = B$  and the problem depends on  $A$  only, which reduces the size of the moment reconstruction problem (i.e. the inversion of the mapping  $A \rightarrow n$ ). This simplification allows to perform one-dimensional numerical simulations on a simple 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. An analytical computation of the closure relations in the case of the full QHD model (as done for the isothermal case) is certainly at reach but need further investigations.

**Appendices.** In these appendices, we write the proofs of several useful lemmas giving relations between the pairs  $(n, nu)$  and  $(A, B)$ , as soon as they are linked according to Definition 2.1.

**Appendix A. Proof of Lemma 2.7.** Consider the following minimization problem with the only constraint of first moment:

$$(A.1) \quad \min \{G(\varrho) \text{ such that } \varrho \text{ is a density operator satisfying (2.1)}\}.$$

Following [10] and with assumptions similar to the ones done in subsection 2.2, this minimization problem (A.1) is attained on a density operator which reads

$$\varrho_0 = (s')^{-1} \left( -\frac{1}{T} H(\alpha, 0) \right),$$

where  $\alpha$  is a scalar function and  $H(\alpha, 0)$  is still defined according to (2.14). Due to the fact that the Wigner function of  $\varrho_0$  is even (see [10]), this density operator carries no current, *i.e.* for any test function  $\Phi$  we have

$$(A.2) \quad -i\hbar \text{Tr} \left\{ \varrho_0 \left( \Phi \cdot \nabla + \frac{1}{2} \text{div} \Phi \right) \right\} = 0.$$

This is enough to conclude that  $\varrho_0 = \varrho_{n,0}^{eq}$  (following Definition 2.1) or, equivalently, that (following the definitions (2.15), (2.16))

$$n(\alpha, 0) = n, \quad (nu)(\alpha, 0) = 0.$$

Denote now

$$\varrho_S = (s')^{-1} \left( -\frac{1}{T} H(\alpha, \nabla S) \right).$$

Applying the Gauge invariance of Lemma 2.3, we have:

$$H(\alpha, \nabla S) = e^{iS/\hbar} H(\alpha, 0) e^{-iS/\hbar},$$

it is immediate to deduce from elementary functional calculus that

$$\varrho_S = e^{iS/\hbar} \varrho_0 e^{-iS/\hbar}.$$

Note then that, by definition, the mass density and the current density corresponding to  $\varrho_S$  are respectively  $n(\alpha, \nabla S)$  and  $(nu)(\alpha, \nabla S)$  and, as a direct consequence of (2.22), we have

$$n(\alpha, \nabla S) = n(\alpha, 0) = n, \quad (nu)(\alpha, \nabla S) = (nu)(\alpha, 0) + n \nabla S = nu.$$

Therefore, according to the property of uniqueness of the Lagrange multipliers  $A$  and  $B$  assumed in subsection 2.2, we deduce that  $A = \alpha$  and  $B = \nabla S$  and the proof is complete.

**REMARK A.1.** Note that we can prove the last part of the lemma,  $n(A, B) = n(A, 0)$ , by a direct computation of the derivative of  $n = \sum_p (s')^{-1} (-\frac{\lambda_p}{T}) |\psi_p|^2$ , (where  $(\lambda_p, \psi_p)_{p \in \mathbb{N}}$  are the eigenelements of the Hamiltonian  $H(A, B)$ ). A perturbation calculus gives us:

$$(A.3) \quad dn(A, B) \cdot (\delta A, \delta B) = \sum_{p, q} T \frac{(s')^{-1}(-\frac{\lambda_p}{T}) - (s')^{-1}(-\frac{\lambda_q}{T})}{\lambda_p - \lambda_q} \operatorname{Re} \left[ \left( \int -\frac{i\hbar}{2} \delta B \cdot \overline{\nabla \psi_q} \psi_p \right. \right. \\ \left. \left. + \frac{i\hbar}{2} \delta B \cdot \nabla \psi_p \overline{\psi_q} + (\delta A + B \cdot \delta B) \psi_p \overline{\psi_q} dx \right) \overline{\psi_p} \psi_q \right],$$

where  $T \frac{(s')^{-1}(-\frac{\lambda_p}{T}) - (s')^{-1}(-\frac{\lambda_q}{T})}{\lambda_p - \lambda_q}$  conventionally equals  $-((s')^{-1})'$  if  $\lambda_p = \lambda_q$ . Now, assume that  $u = B = \nabla S$  and let us note  $\tilde{\psi}_p = e^{-iS/\hbar} \psi_p$ . It is straightforward to check that the sequence  $(\tilde{\psi}_p)_{p \in \mathbb{N}}$  forms an orthogonal basis of real eigenfunctions of the Hamiltonian  $H(A, 0)$ , so that we can write  $\psi_p = e^{iS/\hbar} \tilde{\psi}_p$  with  $\tilde{\psi}_p$  real. Then, substituting this last equality in (A.3) and using the fact that  $B = \nabla S$ , we get:

$$(A.4) \quad dn(A, B) \cdot (\delta A, \delta B) = \sum_{p, q} T \frac{(s')^{-1}(-\frac{\lambda_p}{T}) - (s')^{-1}(-\frac{\lambda_q}{T})}{\lambda_p - \lambda_q} \left( \int \delta A \tilde{\psi}_p \tilde{\psi}_q dx \right) \tilde{\psi}_p \tilde{\psi}_q,$$

and we see that the derivative of the density with respect to  $B$  is zero, so that  $n(A, B) = n(A, 0)$ . Note that we use this property in order to solve our numerical scheme in 1D (see section 4). We use indeed the derivative of the density (A.4) in the Newton algorithm.

**Appendix B. Proof of Lemma 3.1.** In order to perform expansions (3.1) and (3.1), we are going to use the Wigner formalism in which the density and the current density are given according to:

$$(B.1) \quad n = \int \mathcal{E} \exp \left( -\frac{1}{T} \left( \frac{1}{2} (p - B)^2 + A \right) \right) \frac{dp}{(2\pi\hbar)^3},$$

$$(B.2) \quad nu = \int p \mathcal{E} \exp \left( -\frac{1}{T} \left( \frac{1}{2} (p - B)^2 + A \right) \right) \frac{dp}{(2\pi\hbar)^3},$$

where  $\mathcal{E} \exp$  is the quantum exponential  $\mathcal{E} \exp = W \circ \exp \circ W^{-1}$  introduced in [10]. Using Proposition 5.3 of [10] which gives the  $\hbar$  expansion of  $\mathcal{E} \exp(a)$  for an arbitrary symbol



$a$ , we find for the symbol  $-\frac{1}{T} \left( \frac{1}{2}(p-B)^2 + A \right)$  the following expansion:

$$\begin{aligned} \mathcal{E} \exp \left( -\frac{1}{T} \left( \frac{1}{2}(p-B)^2 + A \right) \right) &= \exp \left( -\frac{1}{T} \left( \frac{1}{2}(p-B)^2 + A \right) \right) \left[ 1 + \right. \\ &+ \frac{\hbar^2}{8T^2} \left( -\Delta A + \Delta B \cdot (p-B) + \partial_i B_j (\partial_j B_i - \partial_i B_j) \right) \\ &+ \frac{1}{3T} (\partial_{ij} A - \partial_{ij} B \cdot (p-B) + \partial_i B \cdot \partial_j B) (p_i - B_i) (p_j - B_j) \\ &\left. + \frac{2}{3T} \partial_i B_j (p_i - B_i) (\partial_j A - \partial_j B \cdot (p-B)) + \frac{1}{3T} |\nabla A - \nabla B_j (p_j - B_j)|^2 \right] + \mathcal{O}(\hbar^4), \end{aligned}$$

where  $\partial_i$  denotes the partial derivative  $\partial/\partial x_i$  and where we used Einstein's summation convention. It remains to calculate the integrals (B.1) and (B.2). We use the fact that:

$$\begin{aligned} \int e^{-p^2/(2T)} dp &= (2\pi T)^{3/2}, \\ \int e^{-p^2/(2T)} p_i dp &= 0, \\ \int e^{-p^2/(2T)} p_i p_j dp &= T(2\pi T)^{3/2} \delta_{ij}, \\ \int e^{-p^2/(2T)} p_i p_j p_k dp &= 0, \\ \int e^{-p^2/(2T)} p_i p_j p_k p_l dp &= T^2 (2\pi T)^{3/2} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \end{aligned}$$

and we notice that  $\partial_i B_j (\partial_j B_i - \partial_i B_j) = -|\nabla \times B|^2$  to obtain the expansion of the density:

$$(B.3) \quad n = n_0 e^{-A/T} \left[ 1 + \frac{\hbar^2}{24T} \left( -2\Delta \left( \frac{A}{T} \right) + \left| \nabla \left( \frac{A}{T} \right) \right|^2 - \frac{1}{T} |\nabla \times B|^2 \right) \right] + \mathcal{O}(\hbar^4).$$

In order to calculate the second integral (B.2), we write:

$$\begin{aligned} nu &= \int (p-B) \mathcal{E} \exp \left( -\frac{1}{T} \left( \frac{1}{2}(p-B)^2 + A \right) \right) \\ &\quad + B \mathcal{E} \exp \left( -\frac{1}{T} \left( \frac{1}{2}(p-B)^2 + A \right) \right) \frac{dp}{(2\pi\hbar)^3}, \\ &= \int (p-B) \mathcal{E} \exp \left( -\frac{1}{T} \left( \frac{1}{2}(p-B)^2 + A \right) \right) \frac{dp}{(2\pi\hbar)^3} + nB, \end{aligned}$$

and computing this last integral for a component  $nu_k$ , we obtain:

$$nu_k = nB_k + \frac{\hbar^2}{12} n_0 e^{-A/T} \left( -\partial_i (\partial_k B_i - \partial_i B_k) - \partial_i \left( -\frac{A}{T} \right) (\partial_k B_i - \partial_i B_k) \right) + \mathcal{O}(\hbar^4).$$

Then, we use the fact that  $n = n_0 e^{-A/T} + \mathcal{O}(\hbar^2)$  and that  $A = T \ln n_0 - \ln n + \mathcal{O}(\hbar^2)$  to obtain

$$nu_k = nB_k - \frac{\hbar^2}{12} \partial_i (n(\partial_k B_i - \partial_i B_k)) + \mathcal{O}(\hbar^4)$$

which is nothing else but the component value of the expansion:

$$(B.4) \quad nu = nB - \frac{\hbar^2}{12} \nabla \times (n \nabla \times B) + \mathcal{O}(\hbar^4).$$

The desired expressions of the expansions of  $A$  and  $B$  are a direct consequence of (B.3) and (B.4) noticing that

$$-2\Delta \left( \frac{A}{T} \right) + \left| \nabla \left( \frac{A}{T} \right) \right|^2 = 4 \frac{\Delta \sqrt{n}}{\sqrt{n}} + \mathcal{O}(\hbar^2).$$

**Appendix C. Proof of Lemma 3.7.** The starting point is the following fact remarked in the above proof of Lemma 2.7 (Appendix A). The density operator  $\varrho_{n,0}^{eq}$  realizes the minimum of the problem (A.1), *i.e.* we have

$$G(\varrho_{n,nu}^{eq}) - G(\varrho_{n,0}^{eq}) \geq 0,$$

where we recall that the free energy was defined in (2.11). Since  $G$  is a convex differentiable function of  $\varrho$ , we deduce that

$$dG(\varrho_{n,nu}^{eq}) \cdot (\varrho_{n,nu}^{eq} - \varrho_{n,0}^{eq}) \geq G(\varrho_{n,nu}^{eq}) - G(\varrho_{n,0}^{eq}) \geq 0.$$

Now, by using the expression (2.43) of the derivative of  $G$  with respect to  $\varrho$  and recalling that

$$\varrho_{n,nu}^{eq} = (s')^{-1} \left( -\frac{1}{T} H(A, B) \right),$$

we get

$$\text{Tr} \left\{ (-H(A, B) + \mathcal{H}) (\varrho_{n,nu}^{eq} - \varrho_{n,0}^{eq}) \right\} \geq 0,$$

*i.e.*

$$\text{Tr} \left\{ \left( -ihB \cdot \nabla - \frac{i\hbar}{2} (\text{div} B) + V - A - \frac{1}{2} B^2 \right) (\varrho_{n,nu}^{eq} - \varrho_{n,0}^{eq}) \right\} \geq 0.$$

Therefore, the desired result (3.13) stems directly from (2.1) and (2.2). From the strict convexity of  $s$ , it is clear that this integral vanishes only in the case  $nu \equiv 0$ .

#### REFERENCES

- [1] A. Arnold, J. L. Lopez, P. A. Markowich, and J. Soler, *An analysis of quantum Fokker-Planck models: A Wigner function approach*, Rev. Mat. Iberoamericana **20** (2004), 771–814.
- [2] R. Balian, *From Microphysics to Macrophysics*, Volume 1, Springer, Berlin, 1991.
- [3] I. Burghardt, K. B. Moller, L. S. Cederbaum and E. R. Bittner, *Quantum hydrodynamics: Mixed states, dissipation, and a new hybrid quantum-classical approach*, Int. J. Quant. Chem. **100** (2004), 1153–1162.
- [4] L. L. Chang, L. Esaki and R. Tsu, *Resonant tunneling in semiconductor double barriers*, Appl. Phys. Lett. **24** (1974), 593–595.
- [5] Z. Chen, B. Cockburn, C. Gardner and J. Jerome, *Quantum hydrodynamic simulation of hysteresis in the resonant tunneling diode*, J. Comput. Phys. **117** (1995), 274–280.
- [6] S. Datta, *Nanoscale device modeling: The Green's function method*, Superlattices and Microstructures **28** (2000), 253–278.
- [7] P. Degond and A. El Ayyadi, *A coupled Schrödinger drift-diffusion model for quantum semiconductor device simulations*, J. Comput. Phys. **181** (2002), 222–259.

- [8] P. Degond, S. Gallego, F. Méhats, *An entropic Quantum Drift-Diffusion model for electron transport in resonant tunneling diodes*, to appear in J. Comp. Phys.
- [9] P. Degond, F. Méhats, C. Ringhofer, *Quantum hydrodynamic models derived from the entropy principle*, Contemp. Math. **371** (2005), 107–331.
- [10] P. Degond, F. Méhats, C. Ringhofer, *Quantum energy-transport and drift-diffusion models*, J. Stat. Phys. **118** (2005), no. 3-4, 625–665.
- [11] P. Degond, C. Ringhofer, *Quantum Moment Hydrodynamics and the Entropy Principle*, J. Stat. Phys. **112** (2003), no. 3-4, 587–628.
- [12] S. Gallego, F. Méhats, *Entropic discretization of a quantum drift-diffusion model*, SIAM J. Numer. Anal. **43** (2005), no. 5, 1828–1849.
- [13] C. Gardner, *The quantum hydrodynamic model for semiconductor devices*, SIAM J. Appl. Math. **54** (1994), no. 2, 409–427.
- [14] C. Gardner, C. Ringhofer, *The smooth quantum potential for the hydrodynamic model*, Phys. Rev. E **53** (1996), 157–167.
- [15] C. Gardner, C. Ringhofer, *The Chapman-Enskog Expansion and the Quantum Hydrodynamic Model for Semiconductor Devices*, VLSI Design **10** (2000), 415–435.
- [16] I. Gasser, A. Jüngel, *The quantum hydrodynamic model for semiconductors in thermal equilibrium*, Z. Angew. Math. Phys. **48** (1997), no. 1, 45–59.
- [17] I. Gasser, P. A. Markowich, *Quantum Hydrodynamics, Wigner Transforms and the Classical Limit*, Asympt. Analysis **14** (1997), no. 2, 97–116.
- [18] H. Grubin, J. Kreskovsky, *Quantum moment balance equations and resonant tunneling structures*, Solid State Electr. **32** (1989), 1071–1075.
- [19] A. Jüngel, *Quasi-hydrodynamic semiconductor equations*, Progress in Nonlinear Differential Equations, Birkhäuser, 2001.
- [20] A. Jüngel, D. Matthes, *A derivation of the isothermal quantum hydrodynamic equations using entropy minimization*, Z. Angew. Math. Mech. **85** (2005), 806–814.
- [21] C. D. Levermore, *Moment closure hierarchies for kinetic theories*, J. Stat. Phys. **83** (1996), 1021–1065.
- [22] E. Madelung, *Quantentheorie in hydrodynamischer Form*, Z. Physik **40** (1926), 322–326.
- [23] F. Nier, *A stationary Schrödinger-Poisson system arising from the modeling of electronic devices*, Forum Math. **2** (1990), no. 5, 489–510.
- [24] E. Polizzi, *Modélisation et simulations numériques du transport quantique balistique dans les nanostructures semi-conductrices*, Ph.D. thesis, INSA, Toulouse, 2001.
- [25] E. Polizzi and N. Ben Abdallah, *Self-consistent three dimensional models for quantum ballistic transport in open systems*, Phys. Rev. B, **66** (2002), 245–301.
- [26] E. Wigner, *On the quantum correction for thermodynamic equilibrium*, Phys. Rev. **40** (1932), 749–759.