

Quantum Hydrodynamic models derived from the entropy principle

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Abstract

In this work, we give an overview of recently derived quantum hydrodynamic and diffusion models. A quantum local equilibrium is defined as a minimizer of the quantum entropy subject to local moment constraints (such as given local mass, momentum and energy densities). These equilibria relate the thermodynamic parameters (such as the temperature or chemical potential) to the densities in a non-local way. Quantum hydrodynamic models are obtained through moment expansions of the quantum kinetic equations closed by quantum equilibria. We also derive collision operators for quantum kinetic models which decrease the quantum entropy and relax towards quantum equilibria. Then, through diffusion limits of the quantum kinetic equation, we establish various classes of models which are quantum extensions of the classical energy-transport and drift-diffusion models.

Key words : Density matrix, quantum entropy, quantum moments, local quantum equilibria, quantum Boltzmann operator, quantum BGK operator, quantum hydrodynamics, quantum drift-diffusion, quantum energy-transport

1 Introduction

In this paper, we are interested in establishing the relations between the microscopic and macroscopic descriptions of large-particle quantum systems such as semiconductors or certain classes of plasmas. For classical systems, the situation is quite well understood (even if there remain many open questions). In most instances, the microscopic dynamics of the system is well-described by a kinetic model, such as the Boltzmann equation, while the macroscopic dynamics is modeled by fluid equations such as the Euler, Navier-Stokes or diffusion equations. Of course, there exist more fundamental levels of descriptions such as the N -particle dynamics itself, but we shall not consider these models in the present study.

Following Hilbert [36], Chapman [16] or Enskog [26], many mathematicians and physicists have investigated the relationships between the two levels of descriptions:

the microscopic (kinetic) one and the macroscopic (fluid) one. In particular, the expressions of the transport coefficients of fluid models (such as viscosity or thermal conductivity) can be related with the microscopic theory by means of asymptotic analysis. Central to kinetic theory is the collision operator, which models the mutual interactions between the particles or their interaction with the surrounding environment. The collision operator is the source of entropy dissipation which induces the relaxation of the system towards local thermodynamical equilibrium. Once this relaxation is achieved, the system evolves according to the fluid equations. The transport coefficients depend in an essential way on the collision operator.

A natural question is whether it is possible to establish the same type of connection between microscopic and macroscopic systems in the framework of quantum mechanics. The quantum counterpart of the Boltzmann equation is the quantum Liouville equation (or equivalently the Wigner equation). However, the quantum Liouville equation is restricted to collisionless systems. The derivation of a collisional quantum Liouville equation, which would be a true equivalent of the Boltzmann equation, mostly remains an open question, in spite of a lot of efforts in this direction (see e.g. [3], [4], [5], [14], [27], [28], [41], [50]). Symmetrically, there is no well-accepted macroscopic quantum model, which would play the same role as the Euler or Navier-Stokes equations do in the classical framework. Quantum hydrodynamic theory (also referred to as Bohmian mechanics) has been mostly developed for a single particle system. Its extension to many particle systems faces a closure problem, as many statistical approaches do, although some attempts relying on perturbative expansions may give an answer in some particular cases (see section 3 below for a review of these questions).

The present work is an attempt to partially answer some of the questions raised above. We shall first start with a quantum hydrodynamic theory which relies on an extension of Levermore's moment approach [40] to quantum systems. By doing so, we shall not only derive a system of quantum hydrodynamic equations, but we shall also clarify what we understand as a local quantum equilibrium state, or quantum maxwellian. This definition will allow us to propose new quantum collision operators, which extend the collision operators of classical theory and share the same properties as the latter, namely moment conservation, quantum entropy dissipation and relaxation towards the quantum maxwellian. We shall also investigate diffusive limits of collisional quantum kinetic equations and establish new diffusion-like models which can be viewed as quantum extensions of the classical drift-diffusion or energy-transport models. These models are relevant to the modeling of contemporary quantum semiconductor devices.

The outline is as follows. In section 2, we summarize the major aspects of classical hydrodynamic theories. Then, in section 3, we review the basic quantum concepts that will be useful throughout this paper and briefly discuss the existing quantum hydrodynamic theories. In section 4, we develop our new quantum hydrodynamics framework. The derivation of quantum collision operators is performed in section 5. From these definitions, in section 6, we investigate diffusive limits of the so-defined collisional quantum Liouville equation which allow us to propose new quantum Drift-

Diffusion and Energy-Transport models.

This paper is a review of earlier work essentially published in [22], [23], [24] and [21]. We refer the reader to these papers for more detail. Although different in the details, the approach developed in section 4 and in [22], [23] bears strong analogies with the so-called NESOM theory (Non-Equilibrium Statistical Operator Mechanics) [42], [45], [54].

2 Review of classical hydrodynamic theories

In the classical framework, microscopic models describe the evolution of the phase-space distribution function $f(x, p, t)$ where $x \in \mathbb{R}^d$ is the position, $p \in \mathbb{R}^d$ is the momentum and $t \geq 0$ is the time. The configuration and momentum spaces are supposed to be of dimension d (in practice $d = 1, 2, 3$). The evolution of $f(x, p, t)$ is ruled by the Boltzmann equation:

$$\partial_t f + p \cdot \nabla_x f - \nabla_x V \cdot \nabla_p f = Q(f), \quad (2.1)$$

where $V = V(x, t)$ is the potential and $Q(f)$ is the collision operator. In this work, we shall consider V as a given entity. In practice however, it usually depends on f through e.g. a Poisson equation. The theory that we shall develop in the present work would easily account for this dependency. The collision operator $Q(f)$ takes into account the close interactions of the particles among themselves or with their surrounding. It is usually given according to a complicated expression which will be detailed at section 5. For the time being, we shall leave it unspecified.

Macroscopic models describe the system by means of averaged quantities which depend on the configuration variable x only. These quantities are usually the particle number density $n(x, t)$, the mean velocity $u(x, t)$ and the temperature $T(x, t)$. They evolve according to balance equations such as mass, momentum and energy balance. As an example, we write below the compressible Euler equations which result from these balances:

$$\frac{\partial}{\partial t} \begin{pmatrix} n \\ nu \\ n|u|^2 + 3nT \end{pmatrix} + \nabla_x \cdot \begin{pmatrix} nu \\ nuu + nT \text{Id} \\ (n|u|^2 + 5nT)u \end{pmatrix} = \begin{pmatrix} 0 \\ -n\nabla_x V \\ -nu \cdot \nabla_x V \end{pmatrix}. \quad (2.2)$$

In these equations, the pressure π is taken equal to $\pi = nT$ according to the perfect gas Equation-of-State. A natural question is whether there exists a relation between the Boltzmann equation (2.1) and the Euler system (2.2).

The answer is yes and one way to see it is through the moment method. Indeed, the quantities n , $q = nu$ and $2W = n|u|^2 + 3nT$ are moments of f , i.e. integrals of f with respect to the momentum variable p according to:

$$\begin{pmatrix} n \\ q \\ 2W \end{pmatrix} = \int f \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} dp. \quad (2.3)$$

Therefore, the moment method consists in multiplying the Boltzmann equation (2.1) by 1, p and $|p|^2$ and integrating it with respect to p . This gives:

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

Then, we use conservation properties satisfied by the collision operator:

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

in order to get the following balance equations:

$$\frac{\partial}{\partial t} \begin{pmatrix} n \\ q \\ 2W \end{pmatrix} + \nabla_x \cdot \int f \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} p dp = \begin{pmatrix} 0 \\ -n \nabla_x V \\ -nu \cdot \nabla_x V \end{pmatrix}. \quad (2.4)$$

The drawback of the moment method is that some fluxes cannot be expressed in terms of the conserved variables n, q, W . For instance, the terms $\int f p_i p_j dp$ (for $i \neq j$) in the second equation and $\int f |p|^2 p dp$ in the third equation cannot be expressed in terms of n, q, W . Therefore, the conservation equations as obtained from the moment method are not closed. We need to find a prescription for the distribution function f which allows to compute these quantities in terms of the conserved variables.

For that purpose, Levermore's methodology [40] (see some related work in [46]) consists in using the entropy minimization principle. The entropy minimization problem is stated as follows: Let $n, T \in \mathbb{R}_+, u \in \mathbb{R}^3$ fixed. Find

$$\min\{H(f) = \int f(\ln f - 1) dp \text{ s.t.} \quad (2.5)$$

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

This problem has a unique solution given by the Maxwellian distribution function:

$$M_{n,u,T} = \frac{n}{(2\pi T)^{d/2}} \exp\left(-\frac{|p-u|^2}{2T}\right). \quad (2.6)$$

The parameters n, u and T of the Maxwellian are such that n, nu and $(n|u|^2 + 3nT)/2$ respectively are its density, momentum and energy, i.e.:

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

The insertion of the Maxwellian Ansatz (2.6) into the moment equations (2.4) gives rise to the Euler equations (2.2). If additional moments are retained in the balance equations, such as the pressure tensor $P_{ij} = \int p_i p_j f dp$, the same approach gives rise to the so-called Levermore moment models [40].

We point out the fact that the entropy minimization problem (2.5) is local in space. Indeed, considering a position x , the entropy minimization problem can be formulated and solved given solely the values of (n, u, T) at x , any without any knowledge of these quantities at the other points. The goal is to achieve the same program for quantum systems. As we shall see, this extension is not entirely straightforward because the entropy minimization problem will lose this locality property.

3 A short review of existing quantum hydrodynamic theories

We start with some basic facts about quantum statistical mechanics. The basic object we shall be concerned with is the density operator (see e.g. [6]). For particles evolving in the space \mathbb{R}^d , the density operator ρ is a Hermitian, positive, trace-class operator on the space $L^2(\mathbb{R}^d)$ of complex-valued square-integrable functions on \mathbb{R}^d , such that

$$\text{Tr}\rho = 1. \quad (3.1)$$

Being trace class, ρ is compact and has a complete orthonormal system of eigenfunctions $(\phi_s)_{s \in S}$ associated with the real eigenvalues ρ_s . Furthermore, by the positivity and trace property (3.1), the ρ_s satisfy

$$0 \leq \rho_s \leq 1, \forall s \in S; \quad \sum_{s \in S} \rho_s = 1.$$

Therefore, we can write the action of ρ onto any function $\psi \in L^2(\mathbb{R}^d)$ according to:

$$\rho\psi = \sum_{s \in S} \rho_s (\psi, \phi_s) \phi_s, \quad (3.2)$$

where (ϕ, ψ) denotes the $L^2(\mathbb{R}^d)$ inner product of two functions ϕ and ψ (supposed linear in the first argument and antilinear in the second one). The physical interpretation of ρ is as follows. The ϕ_s describe the possible eigenstates of the system. We are dealing with a large particle system, for which the precise number of particles on each eigenstate is not determined. Therefore, the ρ_s are the probabilities of finding particles on the state labeled by s . Being a probability, ρ_s is comprised between 0 and 1 and the ρ_s must sum up to 1.

In the evolution of the quantum system, each eigenstate ϕ_s evolves according to the Schrödinger equation. We assume that the statistical uncertainty which is encompassed in the ρ_s does not change as time evolves. From these principles, it is an easy matter to show that the density operator evolves according to the following Quantum Liouville equation

$$i\hbar\partial_t\rho = [\mathcal{H}, \rho], \quad (3.3)$$

where \mathcal{H} is the quantum Hamiltonian, i.e. the operator whose action on any function $\psi \in L^2(\mathbb{R}^d)$ is given by:

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

and the brackets stand for the operator commutators $[\mathcal{H}, \rho] = \mathcal{H}\rho - \rho\mathcal{H}$. The real-valued function $V(x, t)$ is the potential acting on the particles (and is supposed known) and \hbar is the reduced Planck constant. So far, the quantum Liouville equation (3.3) describes a non-interacting particle quantum system. Like for the Boltzmann equation, we shall assume that particle interactions (among themselves or with the surrounding) can be described by a collision operator $Q_L(\rho)$ at the right-hand side of (3.3). In other words, we write a collisional quantum Liouville equation as

$$i\hbar\partial_t\rho = [\mathcal{H}, \rho] + i\hbar Q_L(\rho). \quad (3.4)$$

The possible forms of the quantum collision operator $Q_L(\rho)$ will be discussed in section 5. For the time being, we shall leave it unspecified and merely suppose that it correctly accounts for dissipation mechanisms.

We now discuss another representation of quantum statistical problems, by means of the so-called Wigner distribution function. let $\underline{\rho}(x, x')$ denote the integral kernel of the operator ρ . The integral kernel $\underline{\rho}(x, x')$ always exists as a distribution such that ρ acts on any function $\psi \in L^2(\mathbb{R}^d)$ according to

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

From (3.2), a possible expression of $\underline{\rho}$ is

$$\underline{\rho}(x, x') = \sum_{s \in S} \rho_s \phi_s(x) \overline{\phi_s(x')},$$

where the upper bar denotes complex conjugation. Now, we introduce the Wigner transform $W[\rho](x, p)$ of ρ as the function defined on the phase-space (x, p) by:

$$W[\rho](x, p) = \int \underline{\rho}\left(x - \frac{1}{2}\xi, x + \frac{1}{2}\xi\right) e^{i\frac{\xi p}{\hbar}} d\xi. \quad (3.5)$$

The Wigner transform admits an inverse operation named 'Weyl quantization' and which to any function $f(x, p)$ defined on phase-space associates an operator $\rho = W^{-1}(f)$ acting on $L^2(\mathbb{R}^d)$ according to:

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

The function f is referred to as the Weyl symbol of ρ . The Wigner transform and the Weyl quantization are isometries between the space \mathcal{L}^2 of operators such that

$\rho\rho^\dagger$ is trace-class (where ρ^\dagger is the adjoint operator of ρ) and $L^2(\mathbb{R}^{2d})$. Indeed, by Plancherel's formula, it is easily found that

$$\text{Tr}\{\rho\rho^\dagger\} = \int W[\rho](x, p) \overline{W[\rho](x, p)} \frac{dx dp}{(2\pi\hbar)^d}. \quad (3.6)$$

If ρ satisfies the collisionless quantum Liouville equation (3.3), $f = W[\rho]$ satisfies the Wigner equation:

$$\partial_t f + p \cdot \nabla_x f - \Theta^\hbar[V]f = 0, \quad (3.7)$$

where $\Theta^\hbar[V]$ is the operator

$$\Theta^\hbar[V]f = \frac{i}{(2\pi)^d \hbar} \int (V(x + \frac{\hbar}{2}\eta) - V(x - \frac{\hbar}{2}\eta)) f(x, q) e^{i\eta \cdot (p - q)} dq d\eta \quad (3.8)$$

When the collisional Liouville equation (3.4) is considered, a collision operator $Q(w)$ must be added at the right-hand side of (3.7) which is obviously the Wigner transform of $Q_L(\rho)$. The resulting collisional Wigner equation is then written:

$$\partial_t f + p \cdot \nabla_x f - \Theta^\hbar[V]f = Q(f), \quad (3.9)$$

where $Q(f)$ is left unspecified for the time being.

We note that the field operator $\Theta^\hbar[V]$ converges as $\hbar \rightarrow 0$ towards the classical field operator of the Boltzmann equation: $\Theta^\hbar[V]f \rightarrow \nabla_x V \cdot \nabla_p f$.

We now shortly review some of the existing quantum hydrodynamic theories. Quantum hydrodynamics is well-established in the framework of single-particle systems. In this case, the system is represented by a single state associated with the wave-function $\psi(x, t)$ which satisfies the Schrödinger equation:

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

Introducing Madelung's transform, we decompose the complex number ψ into its modulus and its argument:

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

and define $u = \nabla_x S$. Then taking the real and imaginary parts of the Schrödinger equation leads to:

$$\partial_t n + \nabla \cdot (nu) = 0, \quad (3.10)$$

$$\partial_t S + \frac{1}{2}|\nabla S|^2 + V - \frac{\hbar^2}{2} \frac{1}{\sqrt{n}} \Delta \sqrt{n} = 0, \quad (3.11)$$

Taking the gradient, the second equation becomes:

$$\partial_t u + u \cdot \nabla_x u = -\nabla_x (V + V_B), \quad (3.12)$$

$$V_B = -\frac{\hbar^2}{2} \frac{1}{\sqrt{n}} \Delta \sqrt{n}. \quad (3.13)$$

The quantity V_B is called the Bohm potential. Without any specification, the symbol ∇ stands for differentiation with respect to x .

System (3.10), (3.12) appears as the density and momentum conservation equations of the Euler system (2.2) with no pressure term and with the additional Bohm potential term, of order $O(\hbar^2)$. In the classical limit $\hbar \rightarrow 0$, i.e. when $V_B = 0$, this system is often referred to as the pressurless gas dynamics system. In this limit, the momentum equation (3.12) can be solved alone (i.e. does not require the knowledge of n). Once u is known, n can be found as a solution of the density transport equation (3.10). Of course, this decoupling ceases to be possible if the potential V is coupled to n through the Poisson equation for instance. It should be noted that, even in the case of a given external potential V , the addition of the Bohm potential couples the two equations strongly, as the ∇V_B terms involves third derivatives of n .

Similarly, when $\hbar \rightarrow 0$, the phase equation (3.11) reduces to the classical Hamilton-Jacobi equation. The momentum equation (3.12) is equivalent to the phase equation (3.11) only for solutions u which are gradients of a scalar function. The Hamilton-Jacobi equation has been the subject of an immense literature which is impossible to quote exhaustively (see e.g. [44]).

When it comes to many-particle systems, quantum hydrodynamics is not so well established. The starting point is a statistical mixture as described by a density operator ρ . Then, each state s gives rise to its own single-state hydrodynamics system (3.10), (3.11). However, the goal is to obtain a system for averaged quantities over the ensemble of statistical states S . If such averages are performed on the systems (3.10), (3.11) obtained for each state s separately, a closure problem occurs: it is impossible to single out a finite set of averaged quantities over s which gives rise to a closed system of equations. This closure problem is of the same nature as that occurring in the passage from kinetic to hydrodynamic equations in section 2.

Various kinds of closure strategies have been proposed in the literature. For instance, [29] proposes the use of the classical Fourier law relating the heat flux to the gradient of the temperature. In [34], a small temperature asymptotics is performed, since the zero-temperature limit can be understood as the single-particle case. In [30], [31], a Chapman-Enskog expansion of a collisional Wigner equation where the collision term is approximated by a relaxation-time model is developed. Each of these theories lead to different closure relations, with different ranges of validity.

In the present paper, a different approach is used. It does not use any perturbation argument (at least at the hydrodynamic level). The closure Ansatz is defined as the solution of an entropy minimization problem (or maximization according to the convention used in physics) under the constraint of given moments. This approach has been developed in detail in [23] and [22]. It is based on a similar approach as Levermore's methodology for classical systems [40]. It is exposed in more detail in the next section.

4 Quantum Hydrodynamics based on entropy minimization

In this section, our goal is to establish a quantum hydrodynamic theory based on the same methodology as that developed in the classical case in section 2.

We first review the concept of entropy in quantum mechanics. While in classical mechanics, the local value of the entropy at a given point is well-defined (namely by the value at that point of the integral $\int f(\ln f - 1) dv$ where $f = f(x, v, t)$ is the distribution function), such a local definition of the entropy does not exist in quantum mechanics. Indeed, the definition of the quantum entropy refers to the entire system, whose statistical uncertainty is described by the density operator ρ . The entropy being a measure of this uncertainty is naturally expressed in terms of the eigenvalues ρ_s of ρ . It is given by:

$$H[\rho] = \text{Tr}\{\rho(\ln \rho - 1)\} = \sum_{s \in \mathcal{S}} \rho_s(\ln \rho_s - 1). \quad (4.1)$$

The expression $\rho(\ln \rho - 1)$ refers to the operator obtained by acting the function $f(\lambda) = \lambda(\ln \lambda - 1)$ onto ρ by functional calculus i.e. $\rho(\ln \rho - 1)$ has the same eigenbasis as ρ and has eigenvalues $\rho_s(\ln \rho_s - 1)$.

Because of the impossibility to assign a local value to the entropy of a quantum system, the entropy minimization principle has to be global, i.e. its formulation and its solution depend on the values of the moments simultaneously at all points in space.

Let us now review the concept of moments. Like in classical mechanics, we define the moments of the system as the moments of its Wigner distribution. Let us introduce the list of monomials $\mu_0(p) = 1$, $\mu_i(p) = p_i$ ($i = 1, \dots, d$), $\mu_{d+1}(p) = |p|^2$, and the vector of monomials $\mu(p) = (\mu_i(p))_{i=0}^{d+1}$. Let $f(x, p)$ be a Wigner distribution function. Then, its vector of hydrodynamic moments is defined by $m[f] = (m_i[f])_{i=0}^{d+1}$, with

$$m_i[f](x) = \int f(x, p) \mu_i(p) \frac{dp}{(2\pi\hbar)^d}.$$

Of course, $m_0 := n$ is the density, $m_i := q_i$ ($i = 1, \dots, d$) are the components of the momentum flux q , and $m_{d+1} := 2W$ is twice the total energy. The normalizing factor $(2\pi\hbar)^{-d}$ arises from the use of (3.6). Using (3.6) and the concept of observable in quantum mechanics (see e.g. [6]), it is readily seen that these definitions correspond to the quantum concept of local observations of the particle number, momentum and energy at point x .

To derive a moment system, we proceed like in section 2 and take the moments of the Wigner equation (3.9). This leads to:

$$\partial_t m[f] + \nabla_x \cdot \int f \mu p \frac{dp}{(2\pi\hbar)^d} - \int \Theta[V] f \mu \frac{dp}{(2\pi\hbar)^d} = \int Q(f) \mu \frac{dp}{(2\pi\hbar)^d},$$

Now, like in the classical case (see section 2), let us assume that the collision operator satisfies the mass, momentum and energy conservation relations:

$$\int Q(f) \mu dp = 0.$$

Similarly, for the hydrodynamic monomials $\mu(p)$, it turns out that the moments of the quantum field operator coincide with the classical ones, i.e.

$$\int \Theta[V]f \mu \frac{dp}{(2\pi\hbar)^d} = \begin{pmatrix} 0 \\ -n\nabla V \\ -2q \cdot \nabla V \end{pmatrix} := \tilde{\Theta}[V]m[f], \quad (4.2)$$

where, for short, we have denoted by $\tilde{\Theta}[V]m[f]$ the action of the field operator onto the moments. We therefore get:

$$\partial_t m[f] + \nabla_x \cdot \int f \mu p \frac{dp}{(2\pi\hbar)^d} - \tilde{\Theta}[V]m[f] = 0, \quad (4.3)$$

Again, for the same reason as in the classical case (see section 2), a closure problem appears. Indeed, the flux integral $\int f \mu p dp$ at the left-hand side of (4.3) cannot be expressed as a function of the moments $m[f]$. Our goal is now to find an Ansatz for the Wigner distribution function f such that this becomes possible.

Inspired by Levermore's moment method in the classical case (see section 2 and [40]), we use the entropy minimization principle. Since the entropy is now defined globally, i.e. throughout the entire spatial domain, the moment constraints must be prescribed as functions. Therefore, the entropy minimization problem is formulated as follows: Given $m = (m_i(x))_{i=0}^{d+1}$ a $d + 2$ -dimensional vector of functions of x , to find a density operator ρ which realizes

$$\min \left\{ H(\rho) = \text{Tr}\{\rho(\ln \rho - 1)\} \text{ s.t. } \int W[\rho] \mu(p) \frac{dp}{(2\pi\hbar)^d} = m(x), \forall x \in \mathbb{R}^d \right\} \quad (4.4)$$

In this minimization problem, the functional to be minimized is expressed in the density operator representation, while the moment constraints are expressed in the Wigner function representation. To solve this problem, we must express both the functional and the constraints in the same representation. It turns out to be easier to write the moment constraints in the density operator representation. To this aim, we dualize the constraint: let $\lambda(x) = (\lambda_i(x))_{i=0}^{d+1}$ be an arbitrary (vector) test function. We can write the constraint:

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

where $\mu \cdot \lambda = \sum_{i=0}^{d+1} \mu_i \lambda_i$. But, using (3.6), we can convert the left-hand side in the density operator representation and write:

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

Then, the entropy minimization principle can be equivalently formulated as follows: Given a set of moments $m = (m_i(x))_{i=0}^{d+1}$, to solve

$$\begin{aligned} \min\{ H[\rho] = \text{Tr}\{\rho(\ln \rho - 1)\} \quad \text{s. t.} \\ \text{Tr}\{\rho W^{-1}[\mu(p) \cdot \lambda(x)]\} = \int m \cdot \lambda \frac{dx}{(2\pi\hbar)^d}, \quad \forall \lambda = (\lambda_i(x))_{i=0}^N \} \end{aligned} \quad (4.5)$$

The solution of this problem is easily found (see [23] and [22]) and is given by ρ_α such that

$$\rho_\alpha = \exp(W^{-1}[\alpha(x) \cdot \mu(p)]), \quad (4.6)$$

where \exp refers to the operator exponential and the vector valued function $\alpha = (\alpha_i(x))_{i=0}^{d+1}$ is such that $m[W[\rho_\alpha]] = m$. The Wigner transform f_α of ρ_α is such that

$$f_\alpha = W[\rho_\alpha] = \mathcal{E}\text{xp}(\alpha(x) \cdot \mu(p)), \quad (4.7)$$

where $\mathcal{E}\text{xp}$ is the following (nonlinear) operator:

$$\mathcal{E}\text{xp} f = W[\exp(W^{-1}(f))], \quad (4.8)$$

which will be referred to later on as the 'Quantum Exponential'. It is indeed the operator exponential read in terms of the Wigner functions.

Formula (4.7) bears striking analogies with the formula for the classical Maxwellian. Indeed, it is readily seen that the Maxwellian (2.6) can be equivalently written

$$M_\alpha = \exp(\alpha \cdot \mu), \quad (4.9)$$

where the vector $\alpha = (\alpha_i)_{i=0}^{d+1}$ is algebraically related to the vector (n, u, T) . In view of this analogy, we shall refer to functions of the form (4.7) as 'quantum Maxwellians'. However, it should be noted that the relation between the parameters $\alpha(x)$ and the moments $m(x)$ is no more local in position. Indeed, the 'quantum exponentiation operator' (4.8) involves heavily non-local operations such as taking the Wigner and inverse Wigner transforms as well as taking an operator exponential.

Now, by analogy with classical hydrodynamic models (see section 2), quantum hydrodynamic models are obtained by closing the hydrodynamic equations (4.3) by the quantum Maxwellian (4.7) which has moments given by m . In other words, the flux integral $\int f \mu p dp$ is computed by replacing f by the quantum Maxwellian f_α whose parameters α are such that $m[f_\alpha] = m$. It is in fact easier to write the quantum hydrodynamic equations as an evolution system for the parameters $\alpha(x, t)$ than for the moments $m(x, t)$. Indeed, in terms of the α 's, the system is written:

$$\begin{aligned} \partial_t \int \mathcal{E}\text{xp}(\alpha \cdot \mu) \mu dp + \nabla_x \cdot \int \mathcal{E}\text{xp}(\alpha \cdot \mu) \mu p dp - \int \Theta[V] \mathcal{E}\text{xp}(\alpha \cdot \mu) \mu dp \\ = 0 \end{aligned} \quad (4.10)$$

In [40], it is shown that classical moment systems are symmetrizable, and thus, hyperbolic and well-posed (at least locally in time). In the present case, the concept

of hyperbolicity is no longer relevant. Indeed, in spite of its appearance, (4.10) is not a partial differential system. Indeed, both operators $\alpha \rightarrow \int \mathcal{E}xp(\alpha \cdot \mu) \mu dp$ and $\alpha \rightarrow \nabla_x \cdot \int \mathcal{E}xp(\alpha \cdot \mu) \mu p dp$ are non-local operators. It is not clear whether this system is of any known type.

However, there is an indication that this system might be (at least locally) well-posed. This is because there is a dissipated global quantity, namely the entropy. We recall that the quantum entropy is a globally defined (i.e. over the entire space region) quantity by $H[\rho] = \text{Tr}\{\rho(\ln \rho - 1)\}$. Using (3.6), it is possible to express the entropy in terms of the Wigner distribution function $f = W[\rho]$ according to:

$$H[f] = \int f(\mathcal{L}n f - 1) \frac{dx dp}{(2\pi\hbar)^d}, \quad (4.11)$$

where $\mathcal{L}n f$ denotes the quantum logarithm, defined as

$$\mathcal{L}n f = W[\ln(W^{-1}(f))], \quad (4.12)$$

and again, \ln stands for the operator logarithm. We define the fluid entropy $S(m)$ of a moment m by:

$$S(m) = H[\rho_\alpha] = \int \mathcal{E}xp(\alpha \cdot \mu) ((\alpha \cdot \mu) - 1) \frac{dx dp}{(2\pi\hbar)^d}, \quad (4.13)$$

where α and m are such that the quantum Maxwellian of parameters α has moments m , i.e.

$$\int \mathcal{E}xp(\alpha \cdot \mu) \mu dp = m.$$

In [23] and [22], it is shown that $S(m)$ is convex. Let us introduce $\Sigma(\alpha)$, the Legendre dual of S (sometimes called the Massieu-Planck potential). Then, the mapping $\alpha \rightarrow m$ can be inverted by means of S and Σ according to:

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

where, on account that S and Σ are not local functions but instead functionals, $\frac{\delta}{\delta m}$ denotes Gâteaux derivatives. In [23] and [22], it is proved that the quantum hydrodynamic model (4.10) is compatible with the entropy dissipation, i.e. that the entropy $S(m)$ is dissipated along any solution $m(t)$ of (4.10):

$$\partial_t S(m(t)) \leq 0, \quad \forall m(t) \text{ solution of (4.10)}. \quad (4.14)$$

The Quantum Hydrodynamic model (4.10) can be given a more familiar form, closer to the expression of the classical gas dynamics Euler equations (2.2). Indeed, (4.10) can be equivalently written:

$$\partial_t n + \nabla_x \cdot nu = 0, \quad (4.15)$$

$$\partial_t nu + \nabla_x (nuu + \mathbb{P}) = -n \nabla_x V, \quad (4.16)$$

$$\partial_t W + \nabla_x \cdot (Wu + \mathbb{P}u + \mathbb{Q}) = -nu \cdot \nabla_x V, \quad (4.17)$$

where u has been defined as $u = q/n$ and where \mathbb{P} and \mathbb{Q} are the Pressure tensor and heat flux vector respectively given by :

$$\mathbb{P} = \int \mathcal{E}\text{xp}(\alpha \cdot \mu)(p - u)(p - u)dp, \quad (4.18)$$

$$2\mathbb{Q} = \int \mathcal{E}\text{xp}(\alpha \cdot \mu)|p - u|^2(p - u)dp. \quad (4.19)$$

with $\alpha = (\alpha_i(x))_{i=0}^{d+1}$ being such that

$$\int \mathcal{E}\text{xp}(\alpha \cdot \mu)\mu dp = \begin{pmatrix} n \\ nu \\ 2W \end{pmatrix}.$$

Note that we can write

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

where $\alpha_0 = A$, $\alpha_i = B_i$ ($i = 1, \dots, d$) and $\alpha_{d+1} = C$.

In contrast with the classical Euler system (2.2), the relations between the pressure tensor \mathbb{P} and the heat flux vector \mathbb{Q} on the one hand, and the moments (n, u, W) on the other hand are not local ones. Indeed, the values of \mathbb{P} and \mathbb{Q} at a given point x depend on the values of (n, u, W) at any other point. Another difference with the classical case is that the pressure tensor \mathbb{P} may be non-diagonal and the heat flux vector \mathbb{Q} may be non-vanishing. This is because $\mathcal{E}\text{xp}(\alpha \cdot \mu)$ is not obviously an even function of the components $(p - u)_i$ nor an even function of the vector $p - u$ as a whole.

The present approach can be extended to a larger set of moments than just the hydrodynamic ones, giving rise to quantum analogues to the moment hierarchies proposed by Levmore in the classical case [40]. We refer to [22] for the details. Also, in [22], the reader will find some considerations about the inversion of the relation $\alpha \rightarrow m$. In particular, using duality theory in optimization, this problem can be put in the form of an unconstrained maximization problem. Some numerical aspects of this problem are also discussed. The practical development of numerical codes based on these models is in progress.

In the next section, we use the definition of the quantum Maxwellians given by (4.7) in order to propose possible extensions of collision operators of classical kinetic theory to quantum systems.

5 Derivation of quantum collision operators

In this chapter, we discuss the possible forms of the collision operators $Q(f)$ in the classical kinetic equations (2.1) and in the quantum ones (3.9). More detail about the present topic can be found in [24]. Let us first consider classical kinetic theory and discuss the form of the celebrated Boltzmann collision operator, which describes

binary collisions in a rarefied gas. This operator is written (see e.g. [15], [18]):

$$Q(f)(x, p, t) = \int_{p \in \mathbb{R}^d} \int_{\Omega \in \mathbb{S}_+^{d-1}} B(|p - p_1|, \Omega) (f' f'_1 - f f_1) dp_1 d\Omega, \quad (5.1)$$

where \mathbb{S}^{d-1} denotes the $d - 1$ dimensional sphere and \mathbb{S}_+^{d-1} is the subset of \mathbb{S}^{d-1} such that $(p - p_1, \Omega) \geq 0$. We use the following standard notations: $f := f(x, p, t)$, $f_1 := f(x, p_1, t)$, $f' := f(x, p', t)$, $f'_1 := f(x, p'_1, t)$. The momenta p' and p'_1 are related to the momenta p (the current momentum) and p_1 (the variable of integration, which represents the momentum of the collision partner) and to the unit vector Ω by means of the so-called collision relations:

$$p' = p - (p - p_1, \Omega)\Omega, \quad p'_1 = p_1 + (p - p_1, \Omega)\Omega. \quad (5.2)$$

p and p_1 are the momenta of the colliding particles before the collision (pre-collisional momenta) while p' and p'_1 are the post-collisional momenta. Ω is the unit vector in the direction of the bisector of the angle between p and p'_1 . By varying it over the set \mathbb{S}_+^{d-1} , we describe all possible geometric configurations of the post-collisional momenta for given pre-collisional ones p and p_1 . The collision relation is a parametrization of the following two relations which express momentum and energy conservation during a collision:

$$p + p_1 = p' + p'_1, \quad p^2 + p_1^2 = p'^2 + p_1'^2. \quad (5.3)$$

Finally, the function $B(|p - p_1|, \Omega)$ is related to the so-called differential scattering cross-section which carries all the information about the physical nature of the interaction between the particles.

Thanks to the conservation relations (5.3), it can be shown (see e.g. [15], [18]) that the collision operator has the following properties:

(i) it preserves mass, momentum and energy locally, i.e. it satisfies

$$\int Q(f) \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} dp = 0, \quad (5.4)$$

(ii) Its kernel is spanned by the classical Maxwellians (2.6), i.e. we have:

$$Q(f) = 0 \iff \exists (n, u, T) \in \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}_+ \text{ such that } f = M_{n,u,T}, \quad (5.5)$$

where $M_{n,u,T}$ is the classical Maxwellian (2.6).

(iii) Q dissipates the classical entropy, i.e. we have

$$\int Q(f) \ln f df \leq 0, \quad (5.6)$$

for any distribution function f . This last property is nothing but the celebrated Boltzmann's H theorem.

We now turn to quantum theory. Our goal is to see how formula (5.1) can be extended in such a way that the resulting collision operator in the collisional Wigner equation (3.9) has the following properties inspired from properties (i) to (iii) above: (i') Q preserves mass, momentum and energy locally, i.e. it satisfies (5.4) at any point x in space.

(ii') Its Kernel is spanned by the quantum maxwellians f_α given by (4.7), i.e.

$$Q(f) = 0, \forall x \in \mathbb{R}^d \iff \exists \alpha(x) \text{ such that } f = f_\alpha, \forall x \in \mathbb{R}^d. \quad (5.7)$$

(iii') Q dissipates the quantum entropy i.e. we have

$$\int_{x \in \mathbb{R}^d} \int_{p \in \mathbb{R}^d} Q(f) \mathcal{L}n f \, dx \, dp \leq 0. \quad (5.8)$$

As shown in [24], a possible form of such a quantum Boltzmann operator is written as follows:

$$Q(f)(x, p, t) = \int_{p \in \mathbb{R}^d} \int_{\Omega \in \mathbb{S}_+^{d-1}} B(|p - p_1|, \Omega) (A(f)' A(f)'_1 - A(f) A(f)_1) dp_1 \, d\Omega, \quad (5.9)$$

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

$$A(f) = \exp \mathcal{L}n f. \quad (5.10)$$

The conversion operator turns any distribution function f which is the symbol of a positive operator into a positive distribution function. For doing so, it first takes the operator logarithm of f and then takes the classical exponent of the resulting Wigner distribution function.

We cannot provide any justification of the expression (5.9) from first physical principles. However, properties (i')-(iii') appear as quite natural requirements which should be fulfilled by any quantum version of the Boltzmann operator. So far, this is the only justification we can propose for the use of this operator.

A simpler collision model which satisfies the same properties (i)-(iii) as the classical Boltzmann model is the so-called BGK operator. It is written

$$Q(f) = M_f - f, \quad (5.11)$$

where M_f is the classical Maxwellian (2.6) which has the same moments as f , i.e. $M_f = M_{n,u,T}$, where (n, u, T) are determined such that

$$\int (M_f - f) \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} dp = 0. \quad (5.12)$$

Again, a simple extension of this operator to quantum mechanics, which satisfies properties (i')-(iii') is obtained as follows:

$$Q(f) = \mathcal{M}_f - f, \quad (5.13)$$

where now \mathcal{M}_f is the quantum Maxwellian (4.7) which again, has the same moments as f , i.e. $\mathcal{M}_f = f_\alpha$, where the vector $\alpha(x, t)$ is determined such that

$$\int (\mathcal{M}_f - f)\mu(p)dp = 0, \quad (5.14)$$

with $\mu = (1, p, |p|^2)$. In particular, the reader will find in [21] a proof that this operator satisfies the entropy dissipation property (iii').

In the next section, using quantum BGK operators, we investigate diffusive limits of the collisional Wigner equation (3.9) which lead to quantum extensions of the well-established classical Drift-Diffusion and Energy-Transport models.

6 Quantum diffusive models

In some physical situations, momentum is not conserved during collisions. This is the case for carrier transport in semiconductors, which is usually dominated by collisions with phonons. In such situations, the mean momentum of the equilibria vanishes and the limit hydrodynamic model is not adapted to capture the transport properties of the fluid at the macroscopic scale. The motion of the mobile species must be observed at longer time scales and its nature is diffusive.

The Classical Drift-Diffusion model is the most popular diffusive model and has been used since the early days of scientific computing in various areas of physics and engineering (see e.g. [43], [52], etc. for semiconductors and [25], [51], etc. for plasmas and gas discharges). It consists of a mass balance equation for the density, supplemented with a constitutive equation for the mass flux describing the combined effects of diffusion and convection under the field. This model assumes that the temperature of the fluid coincides with that of the surrounding medium. At variance, the Classical Energy-Transport model takes into account the evolution of the temperature. This model, known since the early work [53], involves an additional energy balance equation, where the energy fluxes are also defined by a constitutive equation.

In order to derive Quantum Drift-Diffusion or Energy-Transport models from the collisional Wigner equation (3.9), a change to the diffusive scale is required: one can rescale the current or, equivalently, rescale the time variable. This is the so-called diffusive (or parabolic) scaling. Introducing the following changes of variables and unknowns in the Wigner-Boltzmann equation

$$t' = \varepsilon t, \quad Q' = \varepsilon Q, \quad (6.1)$$

we obtain the rescaled Wigner equation (omitting the primes for simplicity):

$$\varepsilon^2 \partial_t f^\varepsilon + \varepsilon(p \cdot \nabla_x f^\varepsilon - \Theta^{\hbar}[V]f^\varepsilon) = Q(f^\varepsilon). \quad (6.2)$$

To get the limit behavior of f^ε , we now need a specific expression of the collision operator. In the absence of a theory based on first physical principles, we shall choose

the simplest of these operators which satisfies the properties (i')-(iii') of the previous section, namely the quantum BGK operator. It has the expression:

$$Q(f) = \mathcal{M}_f - f, \quad (6.3)$$

where \mathcal{M}_f is the local equilibrium solving the entropy minimization problem with moment constraints associated with f . Moreover, we shall slightly depart from the context described in the previous section, because we want to include collisions of electrons with phonons and lattice defects.

Two situations are studied here. In the first case, Q typically represents the combination of a phonon collision operator in its elastic limit and an electron-electron scattering operator. Such an operator locally preserves the electron number (or local density) and the local energy. It leads to a Quantum Energy-Transport model, where the electron gas is described by two macroscopic quantities: the density and the internal energy. The second case considers an inelastic collision operator (at a longer time scale, the inelastic collision operator with phonons becomes important) and leads to an equilibration of the temperature to the background temperature (temperature of the phonon gas). We derive a Quantum Drift-Diffusion model from (6.1) by prescribing a collision operator which conserves only the local density. For more clarity, we shall treat this model before the Quantum Energy-Transport model. In both cases, the results will be given without proof; all the details can be found in [21].

The diffusion approximation procedure has first been developed in the context of neutron transport (see e.g. [39], [13], [9]) and radiative transfer [7], [8]. Its first application to semiconductors and the rigorous derivation of the Classical Drift-Diffusion model is found in [49], [35]. The Classical Energy-Transport model was derived from the semiconductor Boltzmann equation in [11], [10] (see also the [17], [37]) and has been analyzed in [19], [20].

6.1 The Quantum Drift-Diffusion model

6.1.1 Statement of the model

The Quantum Drift-Diffusion model describes the long term behavior of a quantum system interacting with a thermal bath at a given temperature T_0 . This interaction does not conserve the energy of carriers and the only conserved moment is the local density. The convenient entropy concept to describe such situations is the relative entropy, given by

$$\tilde{H}[\rho] = \int f \left(\mathcal{L}n f - 1 + \frac{h(x, p)}{T_0} \right) \frac{dx dp}{(2\pi\hbar)^d} = \text{Tr} \left\{ \rho \left(\mathcal{L}n \rho - 1 + \frac{\mathcal{H}}{T_0} \right) \right\}, \quad (6.4)$$

with $f = W[\rho]$. In this definition, $\mathcal{H} = -\frac{\hbar^2}{2}\Delta + V$ is the quantum Hamiltonian and $h = W(\mathcal{H})$ is its symbol given by $h(x, p) = \frac{|p|^2}{2} + V$. Remark that $T_0\tilde{H}[\rho]$ is the total free energy of the system.

Now, we consider the problem of minimizing \tilde{H} under the constraint of given density $n(x)$. More precisely, given a density function $n(x)$, we consider the problem:

$$\min \left\{ \tilde{H}[\rho] \mid \int W[\rho](x, p) \frac{dp}{(2\pi\hbar)^d} = n(x) \quad \forall x \in \mathbb{R}^d \right\}. \quad (6.5)$$

Assuming that this minimization problem has a solution, one can express this solution by using the quantum exponential (4.8): this solution is given by $\tilde{\rho}_{\tilde{a}} = W^{-1}[\tilde{f}_{\tilde{a}}]$ with

$$\tilde{f}_{\tilde{a}} = \mathcal{E}\text{xp} \left(\tilde{a}(x) - \frac{h(x, p)}{T_0} \right),$$

where $\tilde{a}(x)$ is such that

$$\int \tilde{f}_{\tilde{a}}(x, p) \frac{dp}{(2\pi\hbar)^d} = n(x) \quad \forall x \in \mathbb{R}^d.$$

Now, with the expression of h , we can write

$$\tilde{f}_{\tilde{a}} = \mathcal{E}\text{xp} \left(\tilde{a}(x) - \frac{V(x)}{T_0} - \frac{|p|^2}{2T_0} \right) = \mathcal{E}\text{xp} \left(a(x) - \frac{|p|^2}{2T_0} \right),$$

with $a = \tilde{a} - V/T_0$. We shall denote the equilibria of this problem by

$$f_a = \mathcal{E}\text{xp} \left(a(x) - \frac{|p|^2}{2T_0} \right), \quad \rho_a = W^{-1}[f_a]. \quad (6.6)$$

We are now able to make the collision operator Q in the Wigner-BGK equation (6.2) precise. It is of the BGK type (6.3), the local equilibrium \mathcal{M}_f associated with f being defined as the quantum Maxwellian (6.6) which has the same density as f :

$$\mathcal{M}_f = \mathcal{E}\text{xp} \left(a - \frac{|p|^2}{2T_0} \right) \quad \text{such that} \quad \int (\mathcal{M}_f - f) dp = 0. \quad (6.7)$$

The diffusion approximation of the Wigner-BGK equation (6.2) is made possible thanks to the following crucial properties of the collision operator:

Lemma 6.1 *The collision operator $Q(f)$ given by (6.3), with \mathcal{M}_f defined by (6.7), has the following properties:*

(i) *Null space:*

$$Q(f) = 0 \iff \exists A(x, t) \text{ such that } f = \mathcal{M}_f = \mathcal{E}\text{xp} \left(A - \frac{|p|^2}{2T_0} \right). \quad (6.8)$$

(ii) *Collisional invariants: For all f , we have:*

$$\int Q(f) dp = 0. \quad (6.9)$$

(iii) *Quantum entropy decay: for all f , we have:*

$$\int Q(f) \left(\mathcal{L}nf + \frac{h}{T_0} \right) dx dp \leq 0, \quad (6.10)$$

with equality if and only if $f = \mathcal{M}_f$

Thanks to these properties, we were able in [21] to make the diffusive approximation of the Wigner-BGK equation (6.2) thanks to a Chapman-Enskog expansion of its solution, which leads to the Quantum Drift-Diffusion model:

Theorem 6.2 *Let f^ε be the solution of the Wigner-BGK equation (6.2), the local equilibria being defined by (6.7). Then, formally, $f^\varepsilon \rightarrow f$ as $\varepsilon \rightarrow 0$, where f is a quantum Maxwellian $f = \mathcal{E}xp(A - |p|^2/(2T_0))$ and $A = A(x, t)$ is a solution of*

$$\partial_t \int \mathcal{E}xp \left(A(x) - \frac{|p|^2}{2T_0} \right) dp - \int \mathcal{T}^2 \mathcal{E}xp \left(A(x) - \frac{|p|^2}{2T_0} \right) dp = 0, \quad (6.11)$$

\mathcal{T} being the quantum transport operator:

$$\mathcal{T}f = (p \cdot \nabla_x - \Theta^{\hbar}[V])f. \quad (6.12)$$

We can write the Drift-Diffusion model in the form of a conservation law. First, for any function $A(x)$, the particle density $n[A]$ associated with A is defined by

$$n[A] = \int \mathcal{E}xp \left(A(x) - \frac{|p|^2}{2T_0} \right) \frac{dp}{(2\pi\hbar)^d}. \quad (6.13)$$

We also introduce the pressure tensor $\Pi[A]$ according to:

$$\Pi[A] = \int p \otimes p \mathcal{E}xp \left(A(x) - \frac{|p|^2}{2T_0} \right) \frac{dp}{(2\pi\hbar)^d}, \quad (6.14)$$

Now, we state:

Lemma 6.3 *The Quantum Drift-Diffusion model (6.11) can be equivalently written:*

$$\partial_t n + \nabla \cdot J = 0, \quad (6.15)$$

where the mass flux J is given by

$$J = -\nabla \cdot \Pi - n\nabla V, \quad (6.16)$$

and Π is a nonlinear functional of n through (6.13) and (6.14).

The Quantum Drift-Diffusion system can be viewed equivalently as an evolution system for A or for n (through the inversion of the non-local relation (6.13)). As a consequence, the implicit relation between Π and n is non-local in space as well. This model is a conservation equation (6.15) for the local density n . The density flux J is given in terms of n through the constitutive relation (6.16). These two equations are formally identical with those involved in the Classical Drift-Diffusion model [17], [11], [10].

At variance, the relation between the pressure tensor and the density is different from the classical one and shows the quantum character of this model. In order

to formally recover the Classical Drift-Diffusion model, it suffices to replace the quantum exponential “ $\mathcal{E}\text{xp}$ ” by the classical one “ exp ” in (6.13), (6.14). Therefore, one can make two comments.

First, the dependence of J upon n is non-local in space. This is due to the non-local character of the functional $\mathcal{E}\text{xp}$, which implies a non-local dependence of Π upon n .

Second, the tensor Π is not diagonal in general. In the classical case, Π is diagonal thanks to the fact that the classical Maxwellian is an even function of each component p_i of p separately. In the quantum case, parity w.r.t. each component p_i of p separately is not preserved by quantum exponentiation (although the parity with respect to p itself is preserved). It follows that, in general, $\mathcal{E}\text{xp}(A + C|p|^2)$ is not an even function of each component of p separately (although $A + C|p|^2$ is, and although $\mathcal{E}\text{xp}(A + C|p|^2)$ is an even function of p as a whole).

An important property satisfied by the Quantum Drift-Diffusion model is the entropy dissipation. More precisely, let us define the quantum relative fluid entropy of the system as:

$$\begin{aligned}\tilde{S}(n) &= \int f_0 \left(\mathcal{L}\mathfrak{n}(f_0) - 1 + \frac{h(x,p)}{T_0} \right) \frac{dp dx}{(2\pi\hbar)^d} \\ &= \int \left(A(x) - 1 + \frac{V}{T_0} \right) \mathcal{E}\text{xp} \left(A(x) - \frac{|p|^2}{2T_0} \right) \frac{dp dx}{(2\pi\hbar)^d} \\ &= \int n \left(A + \frac{V}{T_0} - 1 \right) dx,\end{aligned}$$

where A and n are related through (6.13) and $f_0 = \mathcal{E}\text{xp}(A - |p|^2/2T_0)$. This is a strictly convex functional of n and we have:

Lemma 6.4 *Let A or n solve the Quantum Drift-Diffusion system (6.11). Then the quantum fluid entropy satisfies:*

$$\frac{d}{dt} \tilde{S}(n) \leq \frac{1}{T_0} \int n \partial_t V dx. \quad (6.17)$$

If the potential V is independent of time, then $\tilde{S}(n)$ is a decreasing function of time:

$$\frac{d}{dt} \tilde{S}(n) \leq 0. \quad (6.18)$$

6.1.2 Global equilibria are steady states of the model

The Quantum Drift-Diffusion model can be written in a slightly more explicit form. Indeed, remarking that

$$A(x) - |p|^2/2T_0 = -\frac{h(x,p)}{T_0} + A(x) + \frac{V(x)}{T_0},$$

and recalling that

$$\mathcal{H} = W^{-1}(h) \quad ; \quad \mathcal{T} = \frac{i}{\hbar} W([\mathcal{H}, W^{-1}(\cdot)]),$$

where $[\cdot, \cdot]$ refers to the operator commutator, we can write, with $f_0 = \mathcal{E}xp(A - |p|^2/2T_0)$,

$$\begin{aligned} \mathcal{T}(f_0) &= \frac{i}{\hbar} W \left[\mathcal{H}, \exp \left(-\frac{\mathcal{H}}{T_0} + A(x) + \frac{V(x)}{T_0} \right) \right] \\ &= \frac{i}{\hbar} W [V + AT_0, f_0] = \Theta_{V+AT_0}^{\hbar} f_0. \end{aligned}$$

In deriving this expression, we have used the fact that $[\rho, \exp(\rho)] = 0$ for any ρ , and we have denoted by $\Theta_{V+AT_0}^{\hbar}$ the operator Θ^{\hbar} with V replaced by $V + AT_0$. Then, using (4.2), we deduce that

$$\int \mathcal{T}^2 f_0 \frac{dp}{(2\pi\hbar)^d} = \nabla \cdot \int p \mathcal{T} f_0 \frac{dp}{(2\pi\hbar)^d} = -\nabla \cdot (n \nabla (V + AT_0)).$$

This is enough to deduce the following equivalent form of the Quantum Drift-Diffusion model:

Lemma 6.5 *The Quantum Drift-Diffusion model (6.11) can be equivalently written:*

$$\partial_t n + \nabla \cdot J = 0, \quad (6.19)$$

where the mass flux J is given by

$$J = -n \nabla (V + AT_0), \quad (6.20)$$

and A is a nonlinear functional of n through (6.13).

Now, the steady states of the Quantum Drift-Diffusion model satisfy the elliptic equation:

$$-\nabla \cdot (n \nabla (V + AT_0)) = 0,$$

where A is related to n through (6.13). Global thermodynamic equilibria given by statistical quantum mechanics (see e.g. [6]) are found through the prescription that the current J vanishes. Indeed, if this is the case, $V + AT_0$ is a global constant, which implies that $A = -V/T_0 + C$, where C is a global constant, actually prescribed by the normalization condition $\text{Tr}\{W^{-1}(f_0)\} = 1$. In view of (6.6), the associated distribution function is written:

$$f_0 = \mathcal{E}xp \left(-\frac{h(x, p)}{T_0} + C \right) = W[\exp(-\mathcal{H}/T_0 + C)],$$

which is the standard form of global thermodynamic equilibria. The normalization constant C can be actually be related to the partition function $\ln Z$ of statistical mechanics [6].

6.1.3 $\mathcal{O}(\hbar^2)$ correction to the Classical Drift-Diffusion model

Thanks to semiclassical pseudodifferential calculus, it is possible to formally expand the quantum exponential \mathcal{E}_{xp} in terms of \hbar and to obtain \hbar -expansions of the Quantum Drift-Diffusion model. The quantum Maxwellian given by (6.7) has the following expansion:

$$\mathcal{E}_{\text{xp}} \left(A(x) - \frac{|p|^2}{2T_0} \right) = \exp \left(A(x) - \frac{|p|^2}{2T_0} \right) \left(1 + \frac{\hbar^2}{8T_0} F^{(2)}(A) \right) + \mathcal{O}(\hbar^4), \quad (6.21)$$

where the correction term reads:

$$F^{(2)}(A) = \Delta A + \frac{1}{3} |\nabla A|^2 - \frac{1}{3} (p \otimes p) : \nabla^2 A. \quad (6.22)$$

If we let $\hbar \rightarrow 0$, it is clear that the quantum exponential \mathcal{E}_{xp} formally converges to the classical exponential. As a consequence, at the semiclassical limit $\hbar \rightarrow 0$, we recover the Classical Drift-Diffusion model from the Quantum Drift-Diffusion model.

Most interestingly, one can keep the $\mathcal{O}(\hbar^2)$ term in the expansion (6.21) and drop the $\mathcal{O}(\hbar^4)$ terms. Inserting this approximate expression of \mathcal{E}_{xp} in (6.13) and (6.14), we obtain a local (but differential) relation between n , Π and A . This enables us to write a Classical Drift-Diffusion model with order \hbar^2 corrections. This model turns out to be identical with the classical model corrected by the Bohm potential [33] which has already been quite intensively used in the physics literature [1], [2]. However, the present work is, to our knowledge, the first justification of this model other than by heuristic arguments based on the formal analogy between the hydrodynamic and drift-diffusion models. Also, our approach allows to show that this model is consistent with (quantum) entropy dissipation. More precisely, we can state the:

Theorem 6.6 (i) *Let n^{\hbar} , J^{\hbar} be the solution of the Quantum Drift-Diffusion (QDD) model (6.15), (6.16). Then, we formally have:*

$$n^{\hbar} = n + \mathcal{O}(\hbar^4), \quad J^{\hbar} = J + \mathcal{O}(\hbar^4),$$

where n and J satisfy the Quantum Drift-Diffusion up to order \hbar^2 (QDD₂):

$$\partial_t n + \nabla \cdot J = 0, \quad (6.23)$$

$$J = -T_0 \nabla n - n \nabla (V + V_B[n]), \quad (6.24)$$

and where

$$V_B[n] = -\frac{\hbar^2}{6} \frac{1}{\sqrt{n}} \Delta(\sqrt{n}), \quad (6.25)$$

is the (rescaled) Bohm potential.

(ii) *Let the fluid entropy up to order \hbar^2 be defined by:*

$$\tilde{S}_2[n] = \int_{\mathbb{R}^d} n \left(\ln n - 1 + \frac{V + V_B[n]}{T_0} \right) dx. \quad (6.26)$$

Then, $\tilde{S}_2[n]$ is twice Gâteaux differentiable and strictly convex and we have for any solution n of (6.23), (6.24):

$$\frac{d}{dt} \tilde{S}_2[n] = - \int_{\mathbb{R}^d} \frac{1}{nT_0} |T_0 \nabla n + n \nabla (V + V_B[n])|^2 dx + \int_{\mathbb{R}^d} \frac{n}{T_0} \partial_t V dx \quad (6.27)$$

$$\leq \int_{\mathbb{R}^d} \frac{n}{T_0} \partial_t V dx. \quad (6.28)$$

In particular, if the potential V is independent of time, then the entropy \tilde{S}_2 decays along the solutions of the QDD₂ model.

Note that the Bohm potential (6.25) has been divided by a factor 3 compared with the expression (3.13). The physical explanation of this discrepancy has not been found so far. This system has been mathematically investigated in [12], [32], [47], [48], [38].

6.2 The Quantum Energy-Transport model

In this section, we require of the collision operator that it conserves two moments of f : the density $\int f dp$ and the energy $\int |p|^2 f dp$. Thanks to the entropy principle, this determines the local equilibrium (or quantum Maxwellian) $\mathcal{M}_f(x, p)$ associated with a distribution function $f(x, p)$. Now, we return to the original definition of the quantum entropy:

$$H[\rho] = \text{Tr}\{\rho(\ln \rho - 1)\}, \quad (6.29)$$

where we have denoted $\rho = W^{-1}(f)$. Then \mathcal{M}_f is defined as the solution of the following constrained minimization problem:

$$\min \left\{ H[W^{-1}(g)] \mid \int (g - f)(x, p) \left(\frac{1}{|p|^2} \right) \frac{dp}{(2\pi\hbar)^d} = 0 \quad \forall x \in \mathbb{R}^d \right\}. \quad (6.30)$$

One can write this minimizer as follows:

$$\mathcal{M}_f(x, p) = \text{Exp}(a(x) + c(x)|p|^2), \quad (6.31)$$

where $a(x)$, $c(x)$ are such that

$$\int \mathcal{M}_f(x, p) \left(\frac{1}{|p|^2} \right) \frac{dp}{(2\pi\hbar)^d} = \int f(x, p) \left(\frac{1}{|p|^2} \right) \frac{dp}{(2\pi\hbar)^d} \quad \forall x \in \mathbb{R}^d.$$

We assume that this procedure uniquely determines the local equilibrium \mathcal{M}_f . Then, the corresponding collision operator defined by (6.3) possesses similar properties as those stated in Lemma 6.7:

Lemma 6.7 *The collision operator $Q(f)$ given by (6.3), with \mathcal{M}_f defined by (6.31), has the following properties:*

(i) *Null space:*

$$Q(f) = 0 \iff \exists(A(x, t), C(x, t)) \text{ such that } f = \mathcal{M}_f = \text{Exp}(A + C|p|^2). \quad (6.32)$$

(ii) *Collisional invariants: For all f , we have:*

$$\int Q(f) \left(\frac{1}{|p|^2} \right) dp = 0. \quad (6.33)$$

(iii) *Quantum entropy decay: for all f , we have:*

$$\int Q(f) \mathcal{L}n f dx dp \leq 0, \quad (6.34)$$

with equality if and only if $f = \mathcal{M}_f$.

Now, we state the main result of this section:

Theorem 6.8 *Let f^ε be the solution of the Wigner-BGK equation (6.2), with the local equilibria \mathcal{M}_f defined by (6.31). Then, formally, $f^\varepsilon \rightarrow f$ as $\varepsilon \rightarrow 0$, where f is a quantum Maxwellian $f = \mathcal{E}xp(A + C|p|^2)$ and $(A, C) = (A(x, t), C(x, t))$ are solutions of*

$$\begin{aligned} \partial_t \int \mathcal{E}xp(A + C|p|^2) \left(\frac{1}{|p|^2} \right) dp \\ - \int \mathcal{T}^2 \mathcal{E}xp(A + C|p|^2) \left(\frac{1}{|p|^2} \right) dp = 0; \end{aligned} \quad (6.35)$$

we recall that \mathcal{T} is the quantum transport operator defined in (6.12).

The Energy-Transport model can be written under the form of conservation laws. For any pair of function $(A(t, x), C(t, x))$, we respectively denote by $n[A, C]$, $\mathcal{W}[A, C]$, $\Pi[A, C]$ and $\mathcal{Q}[A, C]$ the particle and energy densities, the pressure tensor and the heat flux tensor associated to A and C , which are defined by

$$\begin{pmatrix} n[A, C] \\ 2\mathcal{W}[A, C] \end{pmatrix} = \int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} \mathcal{E}xp(A + C|p|^2) \frac{dp}{(2\pi\hbar)^d} \quad (6.36)$$

and

$$\begin{pmatrix} \Pi[A, C] \\ 2\mathcal{Q}[A, C] \end{pmatrix} = \int_{\mathbb{R}^d} \begin{pmatrix} p \otimes p \\ |p|^2 p \otimes p \end{pmatrix} \mathcal{E}xp(A + C|p|^2) \frac{dp}{(2\pi\hbar)^d}. \quad (6.37)$$

With these notations, we state:

Lemma 6.9 *The Quantum Energy-Transport model (6.35) can be equivalently written:*

$$\partial_t n + \nabla \cdot J^n = 0, \quad (6.38)$$

$$\partial_t \mathcal{W} + \nabla \cdot J^w + J^n \cdot \nabla_x V = 0, \quad (6.39)$$

where the mass and energy fluxes J^n and J^w are given by

$$J^n = -\nabla \cdot \Pi - n \nabla V, \quad (6.40)$$

$$J^w = -\nabla \cdot \mathcal{Q} - \mathcal{W} \nabla V - \Pi \nabla V + \frac{\hbar^2}{8} n \nabla_x \Delta_x V. \quad (6.41)$$

where Π , \mathcal{Q} are nonlinear functionals of n and \mathcal{W} through (6.36), (6.37).

Theorem 6.8 and Proposition 6.9 enable us to see the Quantum Energy-Transport either as an evolution system (6.35) for the intensive variables (A, C) or as two conservation laws (6.38), (6.39) for the extensive variables (n, \mathcal{W}) . These two formulations are equivalent through the inversion of (6.36), (6.37), this procedure being non-local in space. Remark that the conservation equations (6.38), (6.39) are identical with those involved in the Classical Energy-Transport model [17], [11], [10]. The constitutive equations (6.40), (6.41) are also identical with those of the classical model, except for the term $\frac{\hbar^2}{8} n \nabla_x \Delta_x V$ in (6.41), which is typically quantum. However, the main difference between the classical and quantum models lies in the relation between Π , \mathbb{Q} and n , \mathcal{W} , which is now non-local in position, and in the fact that Π and \mathbb{Q} are not diagonal tensors in general (for the same reason as in the Drift-Diffusion case).

Like the Quantum Drift-Diffusion model, the Quantum Energy-Transport model (6.35) satisfies an entropy dissipation inequality. This property is a direct consequence of our derivation, thanks to the entropy dissipation inequality satisfied by the collision operator (6.34). Denoting $f_0 = \mathcal{E}xp(A + C|p|^2)$, the quantum fluid entropy reads:

$$\begin{aligned} S(n, \mathcal{W}) &= \int f_0 (\mathcal{L}n(f_0) - 1) \frac{dp dx}{(2\pi\hbar)^d} \\ &= \int (A + C|p|^2 - 1) \mathcal{E}xp(A + C|p|^2) \frac{dp dx}{(2\pi\hbar)^d} \\ &= \int (A n + 2C \mathcal{W} - n) dx, \end{aligned} \tag{6.42}$$

where (A, C) and (n, \mathcal{W}) are related through (6.36). In [22], it was proved that S is a strictly convex functional of (n, \mathcal{W}) . Then, we have:

Lemma 6.10 *Let (A, C) or (n, \mathcal{W}) solve the Quantum Energy-Transport system (6.35). Then the quantum fluid entropy $S(n, \mathcal{W})$ is a decreasing function of time:*

$$\frac{d}{dt} S(n, \mathcal{W}) \leq 0. \tag{6.43}$$

7 Conclusion

In this paper, we have presented a new methodology for deriving quantum hydrodynamic and diffusion models. This approach is based on the entropy minimization principle and allows to define the quantum analogues of the classical Maxwellians, which we call quantum Maxwellians. Then, quantum hydrodynamic models can be obtained from a moment expansion of the Wigner equation and a closure Ansatz using these quantum Maxwellians. Using the same methodology, we are able to propose expressions of quantum collision operators of Boltzmann type, and, after a diffusive scaling of the resulting collisional Wigner equation, to derive new quantum diffusion

models of the Drift-Diffusion or Energy-Transport type. The design of appropriate numerical methods for practically solving these models is in progress.

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