Journal of Statistical Physics, Vol. 118, Nos. 3/4, February 2005 (© 2005)
DOI: 10.1007/s10955-004-8823-3

Quantum Energy-Transport and Drift-Diffusion Models

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Received September 29, 2003; accepted September 15, 2004

We show that Quantum Energy-Transport and Quantum Drift-Diffusion models can be derived through diffusion limits of a collisional Wigner equation. The collision operator relaxes to an equilibrium defined through the entropy minimization principle. Both models are shown to be entropic and exhibit fluxes which are related with the state variables through spatially non-local relations. Thanks to an $\hbar$ expansion of these models, $\hbar^2$ perturbations of the Classical Energy-Transport and Drift-Diffusion models are found. In the Drift-Diffusion case, the quantum correction is the Bohm potential and the model is still entropic. In the Energy-Transport case however, the quantum correction is a rather complex expression and the model cannot be proven entropic.

KEY WORDS: Wigner equation; entropy minimization; quantum BGK operator; diffusion approximation.

1. INTRODUCTION

Classical Drift-Diffusion and Energy-Transport models have been invaluable tools for many years in various areas of physics and engineering. They describe the transport of charged-species in strong interaction with a surrounding medium. Such situations occur e.g. in semiconductors (where electrons and holes are interacting with the crystal impurities and the phonons) or in cold plasmas or gas discharges (where the electrons and the ions are interacting with the surrounding neutral molecules).

Drift-Diffusion models have been used since the early days of scientific computation (see e.g. refs. 54, 66, etc. for semiconductors and

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refs. 28, 64, etc. for plasmas and gas discharges). They consist of a mass balance equation for the density of the conductive species, supplemented with a constitutive equation for the mass flux describing the combined effects of convection under the field and diffusion.

The Drift-Diffusion model assumes that the temperature of the mobile species coincides with that of the surrounding medium. This is sometimes too restrictive. The Energy-Transport model involves the temperature of the mobile species as a variable of the problem in addition to the density. The temperature evolves according to an energy balance equation where the energy fluxes are defined by a similar constitutive relation as the mass flux. One can find an account of the recent theory of the Energy-Transport model in ref. 46 in the context of semiconductors.

Classical Drift-Diffusion and Energy-Transport models can be derived from microscopic transport models such as the Boltzmann equation. The passage from the Boltzmann equation to these models, the so-called "diffusion approximation", heavily relies on the description of the interactions between the mobile species and the surrounding medium at the kinetic level by means of the collision operator. To carry the diffusion approximation through, the collision operator must satisfy a certain number of properties, like e.g. space and time locality, the existence of collisional invariants (conserved quantities during a collision) and equilibrium states (the Maxwellians), entropy decay and invertibility in the orthogonal direction to the equilibria.

Currently, the microelectronics industry produces highly miniaturized devices with very small characteristic length scales. In such devices, quantum effects become important and even, sometimes, predominant. A lot of works are devoted to the numerical simulations of quantum transport models in semiconductors (see e.g. refs. 22, 31, 32, 47, 56). Yet, most of these authors do not attempt to adapt Drift-Diffusion and Energy-Transport theories but rather, start from different models. It would seem more efficient to use some adaptation of the former since the existing classical codes could be used as starting bases.

However, this approach is seldom used (see however a quantum version of the Drift-Diffusion model in refs. 2, 3), because it is extremely difficult to perform the derivation of Drift-Diffusion models from the kinetic level in a quantum setting. Indeed, this would require a quantum theory of collisions. Such a theory is still at a rather early stage (see e.g. refs. 4, 19, 29, 51, 63) and more recently refs. 6, 7, 33) and provides collision operators which do not have the properties required in the diffusion approximation process.

The present work is an attempt to partly fill this gap, at least on the formal level. It uses an earlier work(25,26) where quantum equilibria (or quantum Maxwellians) are defined as minimizers of the quantum entropy, subject to **local constraints** of, say, given mass and energy. By local constraints, we mean that we enforce, not only that the total number of particles and the total energy of the system is fixed, like in usual quantum statistical mechanics approaches,$^{(8)}$ but that the local density and energy **at any given point** x are given functions. The result of this constrained minimization problem is that the quantum Maxwellians depend non-locally on the thermodynamic variables (i.e. the Lagrange multipliers of the constraints).

Thanks to the definition of these quantum equilibria, it was possible in ref. 27 to generalize the expression of the collision operators of classical kinetic theory to quantum ones. These operators display the same properties as the classical ones, but for the fact that the equilibria are quantum ones and that they decrease the quantum entropy. In the present work, we introduce simpler operators, of relaxation type (also called 'BGK' operators in the classical framework) which allow more explicit computations than the operators of ref. 27. One of the tasks we shall fulfill is to prove that these operators have the necessary properties for the diffusion approximation to work. The rationale for the use of these simplified operators stems from the analogy with the classical case, where they have been proved to be in a reasonable sense a valuable alternative to the much more complex Boltzmann operator$^{(20)}$.

After the definition of these quantum BGK operator, we follow the standard route defined by the diffusion approximation methodology. Since macroscopic models of Drift-Diffusion or Energy-Transport types are expected to be valid at large scales, we perform a diffusion scaling of the quantum kinetic equation (or Wigner equation). The Quantum Drift-Diffusion and Quantum Energy-Transport models appear at the leading order when we let the scale ratio (often called the Knudsen number in gas dynamics) tend to zero. They differ from their classical counterpart in that the dependence of the (mass and energy) fluxes upon the density and temperature is non-local in space. This is the signature of the non-local dependence of the quantum Maxwellian upon its thermodynamic parameters. An important property is that the entropy decays along any solution of these models. Of course, this property originates from the definition of the quantum Maxwellians through the entropy minimization principle.

In an attempt to find more explicit flux expressions, we study their expansion in powers of the parameter $\hbar$ (this parameter should be viewed as a scaled dimensionless version of the Planck constant $\hbar$). Of course, at leading order when $\hbar \to 0$, we recover the classical models. More interesting is the first order correction, of order $\hbar^2$.

In the case of the Drift-Diffusion model, this correction is shown to involve the so-called Bohm potential, which occurs in many quantum hydrodynamics(38,39,43) and quantum drift-diffusion(2,3) theories. Consequently, this paper gives a way to derive this Quantum Drift-Diffusion model from first principles. We can also show that the Classical Drift-Diffusion model corrected with the Bohm potential remains entropic. To our knowledge, the proof of this property is new. Other mathematical properties and numerical simulations of this model can be found in ref. 17, 61, 62.

In the case of the Energy-Transport model however, the correction to the classical model seems too complex for practical purposes and additionally, we were unsuccessful in trying to prove the entropy property. In the case where we can neglect the temperature gradients compared with the density gradients, the model simplifies slightly.

We conclude this introduction by a few other bibliographical notes. The first macroscopic quantum models that have been derived were of hydrodynamic nature (the difference between hydrodynamic like and diffusion like models will be summarized in section 5.1). The reader will find in refs. 30, 35, 40, 43 a sample of recent works on quantum hydrodynamic models. The entropy minimization principle which is the core of the present work has previously been used to derive quantum hydrodynamic models in refs. 25 and 26. A different, but related approach, can be found in refs. 52, 55, 68. All these approaches rely on methods which, in the classical setting, have been developped in refs. 50, 57.

The diffusion approximation procedure has first been developped in the context of neutron transport (see e.g. refs. 48, 18, 11) and radiative transfer(9,10). Its first application to semiconductors and the rigorous derivation of the Classical Drift-Diffusion model is found in refs. 41, 60. The Classical Energy-Transport model appears in the early work(67). Its first derivation from the semiconductor Boltzmann equation is due to ref. 15 and ref. 13 (see also the ref. 21). It has been analyzed in refs. 23, 24.

The outline of the paper is as follows. In Section 2, we present the starting point of our analysis: the Wigner-BGK model. Then, in Section 3, the diffusion limit leading to the Quantum Energy-Transport model is performed. Section 4 summarizes the same programme for the Quantum Drift-Diffusion model. In Section 5, expansions of the so-obtained models in powers of $\hbar$ are developped. A conclusion is drawn in Section 6 and an appendix collects some useful technical formulae.

Future developments of this work will involve both theoretical investigations (proof of well-posedness, stability, etc.), and numerical ones (simulation of a resonant tunneling diode, for instance). Among the questions which remains to be solved are the establishment of correct boundary conditions for the Quantum Energy-Transport and Quantum Drift-Diffusion models. This implies setting up an entropy minimization problem on a bounded domain with boundary conditions. This question is under investigation in a future work (Gallego and Mishats, submitted)(34). In particular, the treatment of open boundary conditions for the Schrödinger equation has been investigated in refs. 49, 5, 16, 12, 14, 59 Ben Abdallah *et al.*, submitted. Its adaptation to the present framework is in progress.

2. THE WIGNER-BGK MODEL

A quantum particle system can be described by its density operator ρ, which is a positive, hermitian, trace-class operator on a Hilbert space $\mathcal{X}$. If the system consists of a single particle in $\mathbb{R}^d$ ($d=1,2,3$ in practice), subject to a given external potential $V(x,t)$, we have $\mathcal{X}=L^2(\mathbb{R}^d)$, the space of square integrable functions on $\mathbb{R}^d$. In this case, the density operator satisfies the quantum Liouville equation

$$i\hbar\partial_t\rho=[\mathcal{H},\rho], \tag{2.1}$$

where $\mathcal{H}$ is the particle Hamiltonian

$$\mathcal{H}=-\frac{\hbar^2}{2}\Delta+V \tag{2.2}$$

and $[\mathcal{H},\rho]=\mathcal{H}\rho-\rho\mathcal{H}$ is the commutator of $\mathcal{H}$ and ρ. In all this work, we assume that the particle mass is constant and equal to unity.

We shall be concerned with many-particle systems. Our initial postulate is that the system can be modeled by a single-particle density operator ρ satisfying a modified Liouville equation

$$i\hbar\partial_t\rho=[\mathcal{H},\rho]+i\hbar\mathcal{Q}(\rho), \tag{2.3}$$

where the potential V in the Hamiltonian $\mathcal{H}$ can be either an external potential or a mean-field like potential and $\mathcal{Q}(\rho)$ is a collision operator describing the mutual interactions between the particles themselves or between the particles and the surrounding environment. In this sense, (2.3) is an equivalent of the classical Vlasov–Poisson–Boltzmann equation which describes semi-classical charged-particle transport in plasmas or semiconductors for instance.

We shall not dwell on what precise form the potential V should take because the forthcoming developments will be independent of it. On the other hand, the precise form of the collision operator matters. In this paper, we shall use our previous works$^{(25)}$ (see also refs. 26 and 27). In ref. 25 we propose to define quantum local equilibria (or quantum Maxwellians) as minimizers of the quantum entropy functional, subject to given local moment constraints (such as local density, momentum and energy). As opposed to global equilibria, whose definitions are standard (see e.g. ref. 8), these quantum Maxwellians depend on the position variable x through their (non-local) relation to the given moment constraints. In ref. 27, we use these quantum Maxwellians to extend the expression of the classical Boltzmann collision operator to the quantum case.

In this paper, we shall consider a simpler collision operator of BGK type. Classical BGK operators provide a simple relaxation model with similar features as the Boltzmann operator (e.g. local conservation of mass, momentum and energy, entropy decay, etc.). In the present paper, we shall provide an extension of the BGK operator to quantum systems. For the purpose of our present developments, we shall restrict to imposing mass and energy conservation.

It is convenient to introduce the Wigner transform of the density matrix ρ. The Wigner transform maps operators on $L^2(\mathbb{R}^d)$ to symbols, i.e. functions of the classical position and momentum variables $(x, p) \in \mathbb{R}^{2d}$. More precisely, let us define the integral kernel of the operator ρ to be the distribution $\underline{\rho}(x, x')$ such that ρ operates on any function $\psi(x) \in L^2(\mathbb{R}^d)$ as follows:

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

The kernel $\underline{\rho}(x, x')$ can always be defined in the distributional sense. Then, the Wigner transform $W[\rho](x, p)$ is defined by:

$$W[\rho](x, p) = \int_{\mathbb{R}^d} \underline{\rho}\left(x - \frac{1}{2}\eta, x + \frac{1}{2}\eta\right) e^{i\eta\cdot p/\hbar}\, d\eta.$$

We shall denote by $h(x, p) = W[\mathcal{H}]$ the Wigner transform of the Hamiltonian (2.2), i.e.

$$h(x, p) = \frac{|p|^2}{2} + V(x, t), \tag{2.4}$$

which is nothing but the classical Hamiltonian.

The Wigner transform is an isometry between the operator space $\mathcal{L}^2 = \{\rho \,|\, \mathrm{Tr}\,\{\rho\rho^\dagger\} < \infty\}$, (where Tr is the operator trace and $\rho^\dagger$ is the hermitian adjoint of ρ), and the space $L^2(\mathbb{R}^{2d})$. Indeed, as an easy consequence of Plancherel's identity, we have, for two operators ρ and σ in $\mathcal{L}^2$:

$$\mathrm{Tr}\,\{\rho\sigma^\dagger\} = \int W[\rho]\,\overline{W[\sigma]}\,\frac{dx\,dp}{(2\pi\hbar)^d}, \tag{2.5}$$

where the bar means complex conjugation. Therefore, the Wigner transform can be inverted and its inverse, also referred to as the Weyl quantization, is defined for any function $f(x,p)$ as the operator acting on $\psi(x) \in L^2(\mathbb{R}^d)$ as:

$$W^{-1}[f]\psi(x) = (2\pi\hbar)^{-d} \int_{\mathbb{R}^{2d}} f\left(\frac{x+y}{2}, p\right) \psi(y)\, e^{\mathrm{i}p\cdot(x-y)/\hbar}\, dp\,dy. \tag{2.6}$$

The Wigner transform $f(x,p)$ of the density matrix ρ can be viewed as a quantum extension of the classical phase-space Boltzmann distribution function. Note that however $f(x,p)$ is not a positive function, despite the fact that ρ is a positive operator (although f is a real number since ρ is a hermitian operator). Taking the Wigner transform of the collisional Liouville equation (2.3), we find the collisional Wigner equation:

$$\partial_t f + p\cdot\nabla_x f - \Theta[V]f = Q(f), \tag{2.7}$$

where $\Theta[V]$ is the operator

$$\Theta[V]f = \frac{\mathrm{i}}{(2\pi)^d} \int_{\mathbb{R}^{2d}} \frac{V(t, x+\frac{\hbar}{2}\eta) - V(t, x-\frac{\hbar}{2}\eta)}{\hbar}\, f(x,p')\, e^{\mathrm{i}(p-p')\cdot\eta}\, d\eta\, dp' \tag{2.8}$$

and $Q(f)$ is the Wigner transform of the collision operator $\mathcal{Q}(\rho)$. In the semi-classical limit $\hbar \to 0$, $\Theta[V]f$ converges to the usual operator $\nabla_x V \cdot \nabla_p f$. Now our next task is to specify $Q(f)$.

We define the local moments of ρ (such as the local mass, momentum and energy) like in the classical case as the moments of f. Therefore, the local density $n = n(x)$, mean velocity $u(x,t)$ and energy $\mathcal{W} = \mathcal{W}(x)$ are defined by

$$\begin{pmatrix} n(x) \\ nu(x) \\ 2\mathcal{W}(x) \end{pmatrix} = \int f(x,p) \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} \frac{dp}{(2\pi\hbar)^d}. \tag{2.9}$$

In this introduction, we omit the possible dependence upon time. Note that n is rather the density normalized by the total number of particles since $\int n\,dx = \mathrm{Tr}\,\rho = 1$.

The quantum entropy is defined globally for the entire system as

$$H[\rho] = \mathrm{Tr}\,\{\rho(\ln\rho - 1)\}, \tag{2.10}$$

where $\ln\rho$ is the operator logarithm of ρ (i.e. if ρ has eigenvalues ρ_s, then $\ln\rho$ has eigenvalues $\ln\rho_s$ in the same basis). Note that, contrary to the classical case, the quantum entropy is defined globally (i.e. is integrated over the space variable). In refs. 25 and 26, we introduced the concept of local equilibrium (or quantum Maxwellian) as a minimizer of the following constrained problem: $(n(x), \mathcal{W}(x))$ being given, find the minimum of the quantum entropy subject to the constraint that the local density and energy are given by n and $\mathcal{W}$, i.e. find

$$\min\left\{ H[\rho] \quad\Big|\quad \int W[\rho](x,p)\begin{pmatrix}1\\ |p|^2\end{pmatrix}\frac{dp}{(2\pi\hbar)^d} = \begin{pmatrix} n(x)\\ 2\mathcal{W}(x)\end{pmatrix} \quad \forall x\in\mathbb{R}^d\right\}. \tag{2.11}$$

In ref. 26, it is (formally) shown that this minimization problem has a solution given by

$$\rho_{a,c} = \exp(W^{-1}(a(x) + c(x)|p|^2)), \tag{2.12}$$

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

$$\int W[\rho_{a,c}](x,p)\begin{pmatrix}1\\ |p|^2\end{pmatrix}\frac{dp}{(2\pi\hbar)^d} = \begin{pmatrix} n(x)\\ 2\mathcal{W}(x)\end{pmatrix} \quad \forall x\in\mathbb{R}^d.$$

In (2.12), exp refers to the operator exponential, defined in a similar way as the operator logarithm. In the forthcoming developments, we shall write

$$f_{a,c} = W[\rho_{a,c}](x,p) = \mathcal{E}\mathrm{xp}\,(a(x) + c(x)|p|^2), \tag{2.13}$$

where the 'quantum exponential' $\mathcal{E}\mathrm{xp}$ is defined, for any symbol $f(x,p)$ by:

$$\mathcal{E}\mathrm{xp}\, f = W[\exp(W^{-1}(f))].$$

Note that, in (2.13), the functions a and c are to be sought in a class of functions in which the exponential is defined and is a trace-class operator. Determining which classes of functions answer this question is a difficult and still open problem. However, a first step in this direction has been made in refs. 34 (Gallego and Méhats submitted), for a discretized version of the problem. In a similar way, we define the 'quantum logarithm' $\mathcal{L}\mathrm{n}$ by

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

We note that, in view of (2.5) and (2.10), we can write:

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

where $f = W[\rho]$.

Now, for given $f(x, p)$, we define $\mathcal{M}_f$ as the quantum Maxwellian which has the same moments as f, i.e.

$$\mathcal{M}_f = \mathcal{E}\mathrm{xp}\,(a + c|p|^2) \quad \text{such that} \quad \int (\mathcal{M}_f - f) \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp = 0.$$

Throughout this paper, we shall suppose that the two integral constraints fix the two functions a and c in a unique way. Proving this fact is a mathematically challenging problem. However, it can be proved for the discrete case (see ref. 34 Gallego and Méhats, submitted) and the extension of the proof to the continuous setting in under investigation.

The uniqueness of a and c implies that $\mathcal{M}_{\mathcal{M}_f} = \mathcal{M}_f$, i.e. the mapping $f \to \mathcal{M}_f$ is a (nonlinear) projector. Then, we define the collision operator as

$$Q(f) = \mathcal{M}_f - f. \tag{2.14}$$

This collision operator models the interaction of the particle system with a background. The interaction leaves the local number and energy of the particles unchanged and relaxes the distribution towards the quantum Maxwellian $\mathcal{M}_f$. In classical semiconductor kinetic theory, such operators model the combination of electron-phonon scattering (in its elastic limit) and electron–electron scattering (see e.g. refs. 21. 15, 13 for a discussion of this point).

Before going further, we can note the following formal properties of the Wigner-BGK model:

Lemma 2.1 (Formal). Let $f(t)$ be the solution of (2.7), (2.14), if it exists, and let $f_I = f|_{t=0}$. (i) If

$$\int f_I \, \frac{dx\,dp}{(2\pi\hbar)^d} = \mathrm{Tr}\left\{W^{-1}(f_I)\right\} = 1,$$

then, for all time $t > 0$, we have

$$\int f(t,x,p)\, \frac{dx\,dp}{(2\pi\hbar)^d} = \mathrm{Tr}\left\{W^{-1}(f(t))\right\} = 1.$$

(ii) If f_I is positive (in the sense of operators, i.e. $\rho_I = W^{-1}(f_I)$ is a positive operator), then, for all time $t > 0$, $f(t)$ remains positive in this sense.

Proof. Since, by construction, for all f we have

$$\int Q(f)\, \frac{dx\,dp}{(2\pi\hbar)^d} = 0,$$

item (i) stems directly from an integration of (2.7), thanks to the useful identity (3.33) written further. The second point can be more easily seen with the collisional quantum Liouville equation (2.3) satisfied by $\rho(t) = W^{-1}(f(t))$. With our choice of a BGK collision operator, this equation takes the form:

$$\partial_t \rho = -\frac{\mathrm{i}}{\hbar}[\mathcal{H}, \rho] + W^{-1}(\mathcal{M}_f) - \rho\,. \tag{2.15}$$

Assuming that it exists, we denote by $U(t,s)$ the two-parameter family of unitary operators generated by $-\frac{i}{\hbar}\mathcal{H}(t)$, which is such that

$$\forall \psi \in L^2(\mathbb{R}^d) \qquad \frac{d}{dt}U(t,s)\psi = -\frac{\mathrm{i}}{\hbar}\mathcal{H}(t)U(t,s)\psi, \qquad U(s,s)\psi = \psi\,.$$

Let $\sigma(t) = U(-t,0)\, e^t\, \rho(t)\, U(t,0)$. Direct calculations show that this self-adjoint operator σ solves

$$\partial_t \sigma = U(-t,0)\, e^t\, W^{-1}(\mathcal{M}_f)\, U(t,0), \qquad \sigma(0) = \rho(0). \tag{2.16}$$

Since the source term in (2.15) takes the form

$$W^{-1}(\mathcal{M}_f) = \exp(W^{-1}(a + c|p|^2)),$$

it is clearly a positive operator and it is readily seen that $U(-t,0)\, e^t\, W^{-1} (\mathcal{M}_f)\, U(t,0)$ is also a positive operator. Hence, $\rho(0)$ being positive, (2.16) implies that $\sigma(t)$ is positive, as for $\rho(t)$. ▮

In the present paper, we are interested in the large-scale dynamics of the Wigner-Boltzmann equation (2.7) with collision operator (2.14). Unlike(25), where the right scaling was a hydrodynamic one, the relevant scaling here is of diffusion type. This is related with the fact that we enforce only two moment constraints related with mass and energy conservation and that we do not enforce momentum conservation. Therefore, we introduce the following changes of variables

$$t' = \varepsilon t\,, \quad Q' = \varepsilon Q\,, \tag{2.17}$$

and get the rescaled Wigner equation (omitting the primes for simplicity):

$$\varepsilon^2 \partial_t f^\varepsilon + \varepsilon (p \cdot \nabla_x f^\varepsilon - \Theta[V] f^\varepsilon) = Q(f^\varepsilon). \tag{2.18}$$

An estimate of the dimensionless parameter ε can be found from the value μ of the mobility of the material. From it, the mean collision time is $\tau = q^{-1} m \mu \sim 10^{-12}$s, where m is the electron effective mass and q the elementary charge. Then $\varepsilon^2 = \tau/\tau_Q$, where τ_Q is an estimate of the typical time of quantum phenomena. Such a time can be, for instance, a typical life-time of a resonant level in an open device and can be larger than τ be several orders of magnitude.

We are interested in the limit $\varepsilon \to 0$ of the present equation, provided an initial datum $f|_{t=0} = f_I$ is given. This limit is discussed in the next section.

3. DERIVATION OF THE QUANTUM ENERGY-TRANSPORT MODEL

3.1. Statement of the Result

The goal of this section is to prove the following:

Theorem 3.1 (Formal). Let f^ε be the solution of the Wigner-BGK equation (2.18). Then, formally, $f^\varepsilon \to f$ as $\varepsilon \to 0$, where f is a quantum Maxwellian $f = \mathcal{E}\mathrm{xp}\,(A + C|p|^2)$ and $(A, C) = (A(x,t), C(x,t))$ are solutions of

$$\begin{aligned} &\partial_t \int \mathcal{E}\mathrm{xp}\,(A + C|p|^2) \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp \\ &\quad - \int \mathcal{T}^2 \mathcal{E}\mathrm{xp}\,(A + C|p|^2) \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp = 0, \end{aligned} \tag{3.1}$$

and $\mathcal{T}$ is the quantum transport operator:

$$\mathcal{T} f = (p \cdot \nabla_x - \Theta[V]) f \,. \tag{3.2}$$

We can write the Energy-Transport model in a slightly more explicit form. First, we introduce some new notations. For any pair of function $(A(t,x), C(t,x))$, the particle and energy densities $n[A,C]$ and $\mathcal{W}[A,C]$ associated with A and C and which depend nonlinearly and functionally on them are defined by

$$\begin{pmatrix} n[A,C] \\ \mathcal{W}[A,C] \end{pmatrix} = \int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ |p|^2/2 \end{pmatrix} \mathcal{E}\mathrm{xp}\,(A + C|p|^2) \frac{dp}{(2\pi\hbar)^d} \,. \tag{3.3}$$

We also introduce $\Pi[A,C]$ (pressure tensor) and $\mathbb{Q}[A,C]$ (heat flux tensor) according to:

$$\Pi[A,C] = \int_{\mathbb{R}^d} p \otimes p \; \mathcal{E}\mathrm{xp}\,(A + C|p|^2) \frac{dp}{(2\pi\hbar)^d} \,, \tag{3.4}$$

$$\mathbb{Q}[A,C] = \int_{\mathbb{R}^d} \frac{|p|^2}{2} \, p \otimes p \; \mathcal{E}\mathrm{xp}\,(A + C|p|^2) \frac{dp}{(2\pi\hbar)^d} \,. \tag{3.5}$$

Now, we state:

Proposition 3.2. The Quantum Energy-Transport model (3.1) can be equivalently written:

$$\partial_t n + \nabla \cdot J^n = 0 \,, \tag{3.6}$$

$$\partial_t \mathcal{W} + \nabla \cdot J^w + J^n \cdot \nabla_x V = 0 \,, \tag{3.7}$$

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

$$J^n = -\nabla \cdot \Pi - n \nabla V \,, \tag{3.8}$$

$$J^w = -\nabla \cdot \mathbb{Q} - \mathcal{W} \nabla V - \Pi \nabla V + \frac{\hbar^2}{8} n \nabla_x \Delta_x V. \tag{3.9}$$

where n, $\mathcal{W}$, J^n, J^w are nonlinear functionals of A and C through (3.3)–(3.5).

The Quantum Energy-Transport system can be viewed equivalently as an evolution system for (A, C) or for $(n, \mathcal{W})$ (through the inversion of the non-local relation (3.3)). The relations between $(\Pi, \mathbb{Q})$ and (A, C) or $(n, \mathcal{W})$ are non-local in space as well. This model appears as a system of two conservation equations (3.6) and (3.7) for the local density n and energy $\mathcal{W}$. The density and energy fluxes J^n and J^w are given in terms of n and $\mathcal{W}$ through the constitutive relations (3.8) and (3.9). The conservation equations (3.6) and (3.7) are identical with those involved in the Classical Energy-Transport model(21, 15, 13). At variance, the flux relations (3.8) and (3.9) are significantly different in several aspects which we detail below.

First, the relation between (J^n, J^w) and $(n, \mathcal{W})$ is non-local in space, through the non-local dependence of Π and $\mathbb{Q}$ upon $(n, \mathcal{W})$. In the Classical Energy-Transport model, the fluxes are local (linear) combinations of the first-order gradients of $(n, \mathcal{W})$. Therefore, the Quantum Energy-Transport model involves a complete delocalization of the expressions of the fluxes.

Second, the tensors Π and $\mathbb{Q}$ are not diagonal in general. In the classical case, Π and $\mathbb{Q}$ are 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).

Now, we discuss an important property satisfied by the Quantum Energy-Transport model (3.1): entropy dissipation. More precisely, let us define the quantum fluid entropy of the system as in ref. 25. Based on an analogy with the Boltzmann entropy $f(\ln f - 1)$, it is written

$$\begin{aligned} S(n, \mathcal{W}) &= \int f_0(\mathcal{L}\text{n}\,(f_0) - 1)\, \frac{dp\, dx}{(2\pi\hbar)^d} \\ &= \int (A + C|p|^2 - 1)\, \mathcal{E}\text{xp}\,(A + C|p|^2)\, \frac{dp\, dx}{(2\pi\hbar)^d} \\ &= \int (A\, n + 2C\, \mathcal{W} - n)\, dx\,, \end{aligned} \tag{3.10}$$

where (A, C) and $(n, \mathcal{W})$ are related through (3.3) and $f_0 = \mathcal{E}\text{xp}\,(A + C|p|^2)$. In ref. 25, it was proved that S is a strictly convex functional of $(n, \mathcal{W})$. Then, we have:

Proposition 3.3. Let (A, C) or $(n, \mathcal{W})$ solve the Quantum Energy-Transport system (3.1). Then the quantum fluid entropy $S(n, \mathcal{W})$ is a decreasing function of time:

$$\frac{d}{dt} S(n, \mathcal{W}) \leqslant 0. \tag{3.11}$$

Theorem 3.1 and Propositions 3.2 and 3.3 rely on the properties of the collision operator Q, which are collected in the following:

Lemma 3.4. The collision operator $Q(f)$ given by (2.14) has the following properties:

(i) Null space:

$$Q(f)=0 \iff \exists (A(x,t), C(x,t)) \text{ such that } f=\mathcal{M}_f=\mathcal{E}\mathrm{xp}\,(A+C|p|^2). \tag{3.12}$$

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

$$\int Q(f)\begin{pmatrix}1\\|p|^2\end{pmatrix}dp=0. \tag{3.13}$$

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

$$\int Q(f)\mathcal{L}\mathrm{n}\, f\, dx\, dp \leqslant 0, \tag{3.14}$$

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

We shall also need the following intermediate results:

Lemma 3.5. For all f, we have:

$$\int \Theta(f)\begin{pmatrix}1\\p\\|p|^2\end{pmatrix}\frac{dp}{(2\pi\hbar)^d}=\begin{pmatrix}0\\-n\nabla_x V\\-2nu\cdot\nabla_x V\end{pmatrix}, \tag{3.15}$$

where n and u are given by (2.9). Moreover, we have:

$$\int \frac{|p|^2}{2}\, p\ \Theta[V]f\,\frac{dp}{(2\pi\hbar)^d}=-(\mathcal{W}\,\mathrm{Id}+\mathbb{P})\nabla_x V+\frac{\hbar^2}{8}n\nabla_x\Delta_x V, \tag{3.16}$$

where Id is the identity tensor, $\mathcal{W}$ is defined by (2.9) and

$$\mathbb{P}=\int_{\mathbb{R}^d} p\otimes p\, f\,\frac{dp}{(2\pi\hbar)^d},$$

is the pressure tensor.

Lemma 3.6. Let $\rho = W^{-1}[f]$ be a hermitian operator associated with the real-valued symbol $f(x, p)$ and with integral kernel $\underline{\rho}(x, y)$. Then, we have

$$f \text{ even w.r.t. } p \iff \underline{\rho} \text{ symmetric (or real-valued)},$$
$$f \text{ odd w.r.t. } p \iff \underline{\rho} \text{ anti-symmetric (or pure imaginary)},$$

and

$$f \text{ even w.r.t. } p \implies \mathcal{E}\text{xp}\, f \text{ even w.r.t. } p\,.$$

Finally, we recall the following lemma, which was proved in refs. 58, 25:

Lemma 3.7. Let g be a strictly increasing continuously differentiable function defined on $\mathbb{R}_+$. Consider that the function

$$G(\rho) = \mathrm{Tr}\{g(\rho)\}, \tag{3.17}$$

is defined on the space of trace-class positive self-adjoint operators ρ. Then G is Gâteaux differentiable and its Gâteaux derivative $\delta G/\delta\rho$ is given by:

$$\frac{\delta G}{\delta \rho}\delta\rho = \mathrm{Tr}\{g'(\rho)\delta\rho\}. \tag{3.18}$$

We note an immediate corollary of this lemma:

Lemma 3.8. Suppose that $\rho = \rho(s)$ is a continuously differentiable function of the real variable s. Then, $G(\rho(s))$ with G defined by (3.17) is a continously differentiable function from $\mathbb{R}$ to $\mathbb{R}$ and

$$\frac{d}{ds}G(\rho(s)) = \mathrm{Tr}\{g'(\rho(s))\frac{d\rho}{ds}\}, \tag{3.19}$$

The proofs of the main results (Theorem 3.1 and Propositions 3.2 and 3.3) are given in the next section. The proof of the auxilliary lemmas (Lemmas 3.4, 3.5 and 3.6) are deferred to a forthcoming section.

3.2. Proofs of the Main Results

Proof of Theorem 3.1. We assume that $f^\varepsilon \to f_0$ as $\varepsilon \to 0$ and that the convergence holds in a space of smooth functions (in this work, we shall stay at the formal level). We rewrite (2.18) shortly:

$$\varepsilon^2 \partial_t f^\varepsilon + \varepsilon \mathcal{T} f^\varepsilon = Q(f^\varepsilon). \tag{3.20}$$

Then, at leading order, (3.20) implies that $Q(f_0) = 0$. Thus, using (3.12), we deduce that there exists $(A(x,t), C(x,t))$, such that

$$f_0 = \mathcal{E}\mathrm{xp}\,(A + C|p|^2)\,. \tag{3.21}$$

Now, we introduce the following (Chapman–Enskog) expansion:

$$f^\varepsilon = \mathcal{M}_{f^\varepsilon} + \varepsilon f_1^\varepsilon, \tag{3.22}$$

thus defining f_1^ε. Then, clearly:

$$\frac{1}{\varepsilon} Q(f^\varepsilon) = -f_1^\varepsilon.$$

Inserting this expression into (3.20), we get:

$$f_1^\varepsilon = -\mathcal{T} f^\varepsilon + \varepsilon \partial_t f^\varepsilon\,. \tag{3.23}$$

Therefore, as $\varepsilon \to 0$, $f_1^\varepsilon \to f_1$ such that

$$f_1 = -\mathcal{T} f_0\,. \tag{3.24}$$

Next, multipliying (3.20) and using the conservation properties (3.13), we get:

$$\partial_t \int f^\varepsilon \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp + \frac{1}{\varepsilon} \int \mathcal{T} f^\varepsilon \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp = 0. \tag{3.25}$$

Now, using (3.22), we have

$$\mathcal{T} f^\varepsilon = \mathcal{T} \mathcal{M}_{f^\varepsilon} + \varepsilon \mathcal{T} f_1^\varepsilon. \tag{3.26}$$

Let $(A^\varepsilon(x,t), C^\varepsilon(x,t))$ be such that $\mathcal{M}_{f^\varepsilon} = \mathcal{E}\mathrm{xp}\,(A^\varepsilon + C^\varepsilon|p|^2)$. Since, $A^\varepsilon + C^\varepsilon|p|^2$ is an even function of p, thanks to Lemma 3.6, $\mathcal{M}_{f^\varepsilon}$ is even w.r.t. p, and so, $\mathcal{T}\mathcal{M}_{f^\varepsilon}$ is odd w.r.t. p (one can see from (2.8) that if f is even then Θf is odd). It follows that

$$\int \mathcal{T}\mathcal{M}_{f^\varepsilon} \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp = 0. \tag{3.27}$$

Therefore, from (3.25)–(3.27), we deduce that:

$$\partial_t \int f^\varepsilon \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp + \int \mathcal{T} f_1^\varepsilon \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp = 0.$$

Taking the limit $\varepsilon \to 0$ gives

$$\partial_t \int f_0 \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp + \int \mathcal{T} f_1 \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp = 0. \tag{3.28}$$

Inserting the expressions of f_0 and f_1 (Eqs. (3.21) and (3.24)) into (3.28) leads to (3.1), which ends the proof. ▮

Proof of Proposition 3.2. Going back to (3.28), we use the expression of $\mathcal{T}$ and Lemma 3.5 to write:

$$\int \mathcal{T} f_1 \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp = \nabla_x \cdot \int p f_1 \begin{pmatrix} 1 \\ |p|^2 \end{pmatrix} dp + \int f_1 \begin{pmatrix} 0 \\ 2p \end{pmatrix} dp \cdot \nabla_x V. \tag{3.29}$$

We define

$$\begin{pmatrix} J^n \\ J^w \end{pmatrix} = \int \begin{pmatrix} 1 \\ |p|^2/2 \end{pmatrix} p f_1 \frac{dp}{(2\pi\hbar)^d}. \tag{3.30}$$

Then, system (3.6) and (3.7) is nothing but (3.28) written using these notations. Now, inserting (3.24) into (3.30) and using again Lemma 3.5 leads to (3.8) and (3.9). ▮

Proof of Proposition 3.3. We multiply (3.20) by $\mathcal{L}\mathrm{n}\,(f^\varepsilon)$ and integrate with respect to x and p:

$$\int (\mathcal{L}\mathrm{n}\, f^\varepsilon)\partial_t f^\varepsilon \, dx\, dp + \varepsilon^{-1} \int (\mathcal{L}\mathrm{n}\, f^\varepsilon)\mathcal{T} f^\varepsilon \, dx\, dp = \varepsilon^{-2} \int (\mathcal{L}\mathrm{n}\, f^\varepsilon)\, Q(f^\varepsilon)\, dx\, dp.$$

Writing $\rho^\varepsilon = W^{-1}[f^\varepsilon]$ and using Lemma 3.8, we remark that

$$\begin{aligned}\frac{d}{dt}\int f^\varepsilon(\mathcal{L}\mathrm{n}\, f^\varepsilon - 1)\,\frac{dp\,dx}{(2\pi\hbar)^d} &= \frac{d}{dt}\mathrm{Tr}\,\left(\rho^\varepsilon(\ln\rho^\varepsilon - \mathrm{Id})\right)\\ &= \mathrm{Tr}\,\left(\ln\rho^\varepsilon\,\partial_t\rho^\varepsilon\right)\\ &= \int(\mathcal{L}\mathrm{n}\, f^\varepsilon)\partial_t f^\varepsilon\,\frac{dp\,dx}{(2\pi\hbar)^d}\,.\end{aligned}$$

We also note that

$$\begin{aligned}-\mathrm{i}\hbar\int(\mathcal{L}\mathrm{n}\, f^\varepsilon)\mathcal{T} f^\varepsilon\,\frac{dp\,dx}{(2\pi\hbar)^d} &= \int(\mathcal{L}\mathrm{n}\, f^\varepsilon)\,W\left(\mathcal{H}\rho^\varepsilon - \rho^\varepsilon\mathcal{H}\right)\frac{dp\,dx}{(2\pi\hbar)^d}\\ &= \mathrm{Tr}\,\left\{(\ln\rho^\varepsilon)\,[\mathcal{H}\rho^\varepsilon - \rho^\varepsilon\mathcal{H}]\right\}\\ &= \mathrm{Tr}\,\left\{\mathcal{H}\,[\rho^\varepsilon(\ln\rho^\varepsilon) - (\ln\rho^\varepsilon)\rho^\varepsilon]\right\}\\ &= 0\,,\end{aligned}$$

where we used the cyclicity of the trace (i.e. $\mathrm{Tr}\{\rho_1, \dots, \rho_n\}$ is invariant under cyclic permutations of $\{\rho_1, \dots, \rho_n\}$), and the fact that any function of ρ commutes with ρ. Now, from (3.14), we deduce that

$$\frac{d}{dt}\int f^\varepsilon(\mathcal{L}\mathrm{n}\, f^\varepsilon - 1)\,dx\,dp \leqslant 0.$$

To complete the proof, we pass to the limit $\varepsilon \to 0$. This ends the proof of the proposition since f^ε converges to $f_0 = \mathcal{E}\mathrm{xp}\,(A + C|p|^2)$, where (A, C) is the solution of the Quantum Energy-Transport model. ▮

3.3. Proofs of the Auxiliary Lemmas

Proof of Lemma 3.4. Properties (i) and (ii) are obvious. The only property to be proved is (iii) (entropy decay).

Let f be a given distribution function. Then, we can write $\mathcal{M}_f = W[\rho]$ where ρ is the solution of the minimization problem (2.11), in which $(n, \mathcal{W})$ are the moments of f given by (2.9). From ref. 25 and Lemma 3.7, we know that $\rho \to H[\rho]$ is convex and that its derivative is written

$$DH_{\rho_0}(\rho) = \mathrm{Tr}\,\left(\ln(\rho_0)\,\rho\right).$$

Let us now introduce the function

$$\Lambda : \lambda \in [0, 1] \mapsto H\left(W^{-1}((1-\lambda)\mathcal{M}_f + \lambda f)\right).$$

By the chain rule, this function is differentiable and we have

$$\begin{aligned}\frac{d\Lambda}{d\lambda}(\lambda) &= \mathrm{Tr}\left(\ln(W^{-1}((1-\lambda)\mathcal{M}_f+\lambda f))\,W^{-1}(f-\mathcal{M}_f)\right)\\ &= \int \mathcal{L}\mathrm{n}\,((1-\lambda)\mathcal{M}_f+\lambda f)\,(f-\mathcal{M}_f)\,\frac{dp\,dx}{(2\pi\hbar)^d}\,.\end{aligned}$$

Moreover, the convexity of H implies that Λ is also convex. Thus we have

$$\frac{d\Lambda}{d\lambda}(1)\geqslant\Lambda(1)-\Lambda(0),$$

which can also be written

$$\int \mathcal{L}\mathrm{n}\,(f)\,(f-\mathcal{M}_f)\,\frac{dp\,dx}{(2\pi\hbar)^d}\geqslant H(f)-H(\mathcal{M}_f)\geqslant 0\,, \tag{3.31}$$

since $\mathcal{M}_f$ is a minimizer.

Now, the left-hand side of (3.31) vanishes identically if and only if $H(f)=H(\mathcal{M}_f)$ which is equivalent to saying that $f=\mathcal{M}_f$ since we assumed that the minimizer $\mathcal{M}_f$ is unique. This ends the proof of *(iii)* and of Lemma 3.4. ▮

Proof of Lemma 3.5. Denoting the Fourier transform with respect to the p-variable by $\widehat{\cdot}$, the operator $\Theta[V]$ is such that

$$\widehat{\Theta[V]f}=\mathrm{i}\frac{V(t,x+\frac{\hbar}{2}\eta)-V(t,x-\frac{\hbar}{2}\eta)}{\hbar}\,\widehat{f}(t,x,\eta). \tag{3.32}$$

Therefore, for smooth enough functions V and f decaying fast enough at infinity, we have the following useful identities:

$$\int_{\mathbb{R}^d}\Theta[V]f\,dp=(2\pi)^d\,\widehat{\Theta[V]f}\,(t,x,0)=0, \tag{3.33}$$

$$\begin{aligned}\int_{\mathbb{R}^d}p\,\Theta[V]f\,dp &= i(2\pi)^d\,\nabla_\eta\,\widehat{\Theta[V]f}\,(t,x,0)\\ &= -(2\pi)^d\nabla_x V(t,x)\cdot\widehat{f}(t,x,0)\\ &= -\nabla_x V\cdot\int_{\mathbb{R}^d}f\,dp,\end{aligned} \tag{3.34}$$

$$\begin{aligned}\int_{\mathbb{R}^d} \frac{|p|^2}{2}\,\Theta[V]f\,dp &= -\frac{1}{2}(2\pi)^d\,\Delta_\eta\,\widehat{\Theta[V]f}\,(t,x,0)\\ &= -i\,(2\pi)^d\nabla_x V(t,x)\cdot\nabla_\eta \widehat{f}(t,x,0)\\ &= -\nabla_x V\cdot\int_{\mathbb{R}^d} pf\,dp\end{aligned} \tag{3.35}$$

and some straightforward calculations lead to (3.16). This concludes the proof of Lemma 3.5. ▌

Proof of Lemma 3.6. The first two statements obviously follow from a change $p \to -p$ in (2.6). We now prove that the parity is preserved in taking the quantum exponential. Let $\underline{\rho}$ be the integral kernel of $W^{-1}f$ and suppose that $\underline{\rho}$ is real-valued. Then, the integral kernel of ρ^2 is

$$\underline{\rho^2}(x,y) = \int \underline{\rho}(x,z)\underline{\rho}(z,y)\,dz,$$

and is also real-valued. Similarly, by induction, the integral kernel of any power of ρ is real valued. Therefore, $\exp\rho$ being the sum of a series of powers of ρ, its integral kernel is also real valued, from which we conclude that $\mathcal{E}\mathrm{xp}\ f$ is even w.r.t. p. ▌

4. DERIVATION OF THE QUANTUM DRIFT-DIFFUSION MODEL

This section is devoted to the derivation of the Quantum Drift-Diffusion model. The Quantum Drift-Diffusion model describes the long term behaviour of a quantum system interacting with a thermal bath at a given temperature. Therefore, the energy of the quantum system is not locally (neither globally) conserved. The resulting model consists of a single conservation equation for the particle density only, with an instantaneous (but non-local in space) relation between the particle current and the density. By contrast, in the Quantum Energy-Transport model, the energy is locally conserved, which implies that the temperature evolves according to the energy balance equation. The resulting model, as we have seen in the previous section, is a system of conservation equations for the density and the energy.

The starting point for the derivation of the Quantum Drift-Diffusion model is again the quantum Boltzmann equation (2.18), but with a different collision operator, which we are now going to introduce.

First, we introduce the convenient entropy concept for systems interacting with a thermal bath at a given temperature T_0. This is the so-called relative entropy, given by:

$$\begin{aligned}\widetilde{H}[\rho] &= \int f(\mathcal{L}\mathrm{n}\, f - 1 + \frac{h(x,p)}{T_0})\, \frac{dx\, dp}{(2\pi\hbar)^d},\\ &= \mathrm{Tr}\{\rho(\ln\rho - 1 + \frac{\mathcal{H}}{T_0})\},\end{aligned} \tag{4.1}$$

with $f = W[\rho]$. We recall the $\mathcal{H}$ is the quantum Hamiltonian (2.2) and h its symbol (2.4).

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

$$\min\{\widetilde{H}[\rho] \quad | \quad \int W[\rho](x,p)\, \frac{dp}{(2\pi\hbar)^d} = n(x) \quad \forall x \in \mathbb{R}^d\}. \tag{4.2}$$

Assuming that this minimization problem has a solution, this solution is given by $\tilde{\rho}_{\tilde{a}} = W^{-1}[\tilde{f}_{\tilde{a}}]$ with

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

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 (2.4) we can write

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

with $a = \tilde{a} - V/T_0$. We shall denote

$$f_a = \mathcal{E}\mathrm{xp}\left(a(x) - \frac{|p|^2}{2T_0}\right), \quad \rho_a = W^{-1}[f_a], \tag{4.3}$$

the equilibria of this problem.

Now, for given $f(x,p)$, we define $\widetilde{\mathcal{M}}_f$ as the quantum maxwellian (4.3) which has the same density as f, i.e.

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

We shall suppose that the integral constraint fixes the function a in a unique way. Then, we define the collision operator as

$$\widetilde{Q}(f) = \widetilde{\mathcal{M}}_f - f. \tag{4.4}$$

This collision operator models the interaction of the particle system with a background of fixed temperature T_0. The interaction leaves the local number of particles unchanged and relaxes the distribution towards the quantum Maxwellian $\widetilde{\mathcal{M}}_f$. In classical semiconductor kinetic theory, this operator would model electron–phonon scattering (without taking the elastic limit) while electron-electron scattering is neglected(13,15,21). (refer to the end of Section 2 for a comparison with the Energy-Transport case).

In this section, we shall perform a diffusion approximation of the Wigner-BGK equation (3.20), i.e.

$$\varepsilon^2 \partial_t f^\varepsilon + \varepsilon \mathcal{T} f^\varepsilon = \widetilde{Q}(f^\varepsilon). \tag{4.5}$$

where now, the BGK-like collision operator $\widetilde{Q}$ is given by (4.4). We only state the results: the proofs are very similar to those concerning the Energy-Transport model.

Theorem 4.1 (Formal). Let f^ε be the solution of the Wigner-BGK equation (4.5). Then, formally, $f^\varepsilon \to f$ as $\varepsilon \to 0$, where f is a quantum Maxwellian $f = \mathcal{E}\mathrm{xp}(A - |p|^2/(2T_0))$ and $A = A(x,t)$ is a solution of

$$\partial_t \int \mathcal{E}\mathrm{xp}\left(A(x) - \frac{|p|^2}{2T_0}\right) dp - \int \mathcal{T}^2 \mathcal{E}\mathrm{xp}\left(A(x) - \frac{|p|^2}{2T_0}\right) dp = 0, \tag{4.6}$$

where we recall that $\mathcal{T}$ is the quantum transport operator (3.2).

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

$$n[A] = \int \mathcal{E}\mathrm{xp}\left(A(x) - \frac{|p|^2}{2T_0}\right) \frac{dp}{(2\pi\hbar)^d}. \tag{4.7}$$

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

$$\Pi[A]=\int p\otimes p\ \mathcal{E}\mathrm{xp}\left(A(x)-\frac{|p|^2}{2T_0}\right)\frac{dp}{(2\pi\hbar)^d}, \tag{4.8}$$

Now, we state:

Proposition 4.2. The Quantum Drift-Diffusion model can be equivalently written:

$$\partial_t n+\nabla\cdot J=0\,, \tag{4.9}$$

where the mass flux J is given by

$$J=-\nabla\cdot\Pi-n\nabla V\,, \tag{4.10}$$

and n and Π are nonlinear functionals of A through (4.7) and (4.8).

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 (4.7)). The relations between Π and A or n are non-local in space as well. This model is a conservation equation (4.9) for the local density n. The density flux J is given in terms of n through the constitutive relation (4.10). These two equations are formally identical with those involved in the Classical Drift-Diffusion model(13,15,21). However, the difference is in the relation between Π and n, which is non-local in the quantum case, and in the fact that Π is not a diagonal tensor in general (for the same reason as in the Energy-Transport case).

The Drift-Diffusion model satisfies an entropy dissipation property. More precisely, let us define the quantum relative fluid entropy of the system as:

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

where A and n are related through (4.7) and $f_0=\mathcal{E}\mathrm{xp}\,(A-|p|^2/2T_0)$. Then, we have:

Proposition 4.3. Let A or n solve the Quantum Drift-Diffusion system (4.6). Then the quantum fluid entropy satisfies:

$$\frac{d}{dt}\widetilde{S}(n) \leqslant \frac{1}{T_0}\int n\,\partial_t V\,dx. \tag{4.11}$$

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

$$\frac{d}{dt}\widetilde{S}(n) \leqslant 0. \tag{4.12}$$

Like for the Energy-Transport model, these results rely on the following properties of $\widetilde{Q}$, the proof of which is a straightforward extension of that of Lemma 3.4.

Lemma 4.4. The collision operator $\widetilde{Q}(f)$ given by (4.4) has the following properties:

(i) Null space:

$$\widetilde{Q}(f) = 0 \quad \Longleftrightarrow \quad \exists A(x,t) \text{ such that } f = \widetilde{\mathcal{M}}_f = \mathcal{E}\mathrm{xp}\left(A - \frac{|p|^2}{2T_0}\right). \tag{4.13}$$

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

$$\int \widetilde{Q}(f)\,dp = 0. \tag{4.14}$$

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

$$\int \widetilde{Q}(f)\left(\mathcal{L}\mathrm{n}\, f + \frac{h}{T_0}\right) dx\,dp \leqslant 0, \tag{4.15}$$

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

We note that, since $\widetilde{\mathcal{M}}_f$ is a minimizer of the relative entropy (4.1), we need to add a term h/T_0 to the entropy inequality (4.15). This term is the reason for the appearence of a right-hand side to the entropy inequality (4.11), which only vanishes if V is independent of time. In the case where V is related with n through the Poisson equation:

$$-\Delta V = n + D, \tag{4.16}$$

where D is a given time independent background charge density, this term is a total time derivative:

$$\frac{1}{T_0}\int n\,\partial_t V\,dx = \frac{1}{2T_0}\frac{d}{dt}\int |\nabla(V+V_0)|^2\,dx\,,$$

with $\Delta V_0 = D$. In that case, we recover the perfect decay of the quantity

$$\int \left(nA - n + \frac{1}{2T_0}|\nabla V|^2\right)\,dx.$$

5. EXPANSIONS IN POWERS OF $\hbar$

5.1. Statement of the Results

The goal of this section is to relate the Quantum Energy-Transport (QET) and Quantum Drift-Diffusion (QDD) models with their classical counterparts (the Classical Energy-Transport (CET) and Classical Drift-Diffusion (CDD) models) through the $\hbar \to 0$ limit. We also aim at finding the leading order correction to these classical models in an expansion in powers of $\hbar$ (i.e. terms of order $\hbar^2$). The so-obtained models will be called the Quantum Energy-Transport up to order $\hbar^2$ (QET$_2$) and Quantum Drift-Diffusion up to order $\hbar^2$ (QDD$_2$). This approach can be viewed as an application of the semi-classical method (see e.g. refs. 1, 44, 45, 65) which has been illustrated in the non-linear case in the work by Grenier(42).

The QDD$_2$ model turns out to be identical with the classical CDD model corrected by the Bohm potential(39). The Bohm potential usually appears in the context of Quantum Hydrodynamic models. For the sake of completeness, let us briefly review this theory.

Starting from the Schrödinger equation

$$i\hbar\partial_t\psi = \mathcal{H}\psi,$$

with $\mathcal{H}$ being the Hamiltonian (2.2), we use the Madelung transformation $\psi = \sqrt{n} \exp \mathrm{i}S/\hbar$ where the density n and the phase S are real-valued functions of (x, t). Inserting this expression into the Schrödinger equation and taking real and imaginary parts, we are led to the following system of equations:

$$\partial_t n + \nabla \cdot (nu) = 0\,, \tag{5.1}$$

$$\partial_t S + \frac{1}{2}|\nabla S|^2 + V + \mathcal{V}_B[n] = 0, \tag{5.2}$$

where

$$\mathcal{V}_B[n] = -\frac{\hbar^2}{2}\frac{1}{\sqrt{n}}\Delta(\sqrt{n}), \tag{5.3}$$

is the so-called Bohm potential and $u = \nabla S$ is the velocity. Eq. (5.1) is the mass convection equation under the velocity u while (5.2) is the classical Hamilton–Jacobi equation perturbed by the Bohm potential $\tilde{V}_B$, which is a correction of order $\hbar^2$.

Taking the gradient of (5.2), we obtain the momentum conservation equation:

$$\partial_t u + u \cdot \nabla u + \nabla(V + \mathcal{V}_B[n]) = 0, \tag{5.4}$$

System (5.1), (5.4) is the system of pressureless Euler equations with, added to the external potential V, the quantum mechanical contribution $\tilde{V}_B$. However, it should be bore in mind that this system is equivalent to the single-particle Schrödinger equation, and as such, does not apply to many-particle systems. To cure this defficiency, one should add other terms to the momentum equation (5.4) (such as pressure, viscosity, etc.) and derive an energy balance equation. One finds in the literature several attemps to realize this programme by introducing some statistical averages over mixed quantum states(40, 30, 35–37). However, a major obstacle on this way is the question of closing the so-obtained chain of statistical equations. In ref. 25 it has been proposed that the closure Ansatz should use Quantum Maxwellians as defined in the present work.

However, our aim here is the derivation of diffusion rather than hydrodynamic models. Diffusion models differ from hydrodynamic ones in the fact that the velocity (or the flux) is prescribed in terms of the other state variables of the problem at all times (see e.g. (3.8) or (4.10)), rather than given through a time-differential relation like in (5.4). The derivation of diffusion models from kinetic ones involves a diffusion scaling like (2.17) rather than a hydrodynamic one (where the same power of ε appears in the scaling of x and t). Therefore, the limits are different. However, it turns out that the same Bohm potential term appears as the leading order quantum correction term to the classical Drift-Diffusion model. This is related with the fact that drift-diffusion models can be derived from relaxed quantum hydrodynamic systems under a diffusive scaling. We simply note that our approach gives rise to a discrepancy of a factor 1/3 to the Bohm potential term which would be obtained by such a method (see (5.7)). So far, there is no physical expanation to this discrepancy.

The Classical Drift-Diffusion system corrected with the Bohm potential has already been used in the physics or mathematics literature(2,3,17,61,62). Our approach provides another derivation of this model. As a by-product of our theory, we also prove that the QDD$_2$ model is entropic. More precisely, expanding the entropy functional S_T in powers of $\hbar^2$ and retaining terms up to order $\hbar^2$, we find an approximate quantum entropy functional, which is still convex and which decays along solutions of the QDD$_2$ model.

We now turn to the statement of the main results concerning the QDD$_2$ model.

Theorem 5.1. (i) Let $n^{\hbar}$, $J^{\hbar}$, the solution of the Quantum Drift-Diffusion (QDD) model (4.9) and (4.10). Then, we formally have:

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

where n and J satisfy the Quantum Drift-Diffusion up to order $\hbar^2$ (QDD$_2$):

$$\partial_t n + \nabla \cdot J = 0, \tag{5.5}$$

$$J = -T_0 \nabla n - n \nabla (V + V_{\mathrm{B}}[n]), \tag{5.6}$$

and where

$$V_B[n] = \frac{1}{3} \mathcal{V}_{\mathrm{B}}[n] = -\frac{\hbar^2}{6} \frac{1}{\sqrt{n}} \Delta(\sqrt{n}), \tag{5.7}$$

is the rescaled Bohm potential.

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

$$\widetilde{S}_2[n] = \int_{\mathbb{R}^d} n(\ln n - 1 + \frac{V + V_{\mathrm{B}}}{T_0})\, dx. \tag{5.8}$$

Then, $\widetilde{S}_2[n]$ is twice Gâteaux differentiable and strictly convex and we have for any solution n of (5.5) and (5.6):

$$\frac{d}{dt}\widetilde{S}_2[n] = -\int_{\mathbb{R}^d} \frac{1}{nT_0}|T_0\nabla n + n\nabla(V + V_B[n])|^2\,dx + \int_{\mathbb{R}^d} \frac{n}{T_0}\partial_t V\,dx \quad (5.9)$$

$$\leqslant \int_{\mathbb{R}^d} \frac{n}{T_0}\,\partial_t V\,dx. \quad (5.10)$$

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

Like at the end of section 4, we remark that, if V is related with n through the Poisson equation (4.16), the following quantity decays in time:

$$\int \left(n\ln n - n + \frac{1}{2T_0}|\nabla(V+V_0)|^2 + \frac{\hbar^2}{6T_0}|\nabla\sqrt{n}|^2 \right) dx.$$

If we let $V_B = 0$ in (5.5) and (5.6) we recover the classical CDD model. Of course, in this model, T_0 is a constant: the temperature of the system is the same as the lattice temperature. However, if we expand the pressure tensor given by (4.8) with respect to $\hbar$ (Eq. (5.33)) and compute the quantity $T^{\hbar} = \mathrm{Tr}\ \Pi^{\hbar}/(dn^{\hbar})$, we get

$$T^{\hbar} = T_0 - \frac{\hbar^2}{12d}\Delta \ln n^{\hbar} + \mathcal{O}(\hbar^4).$$

Therefore, a generalized temperature for the QDD$_2$ system can be defined by $T = T_0 - \frac{\hbar^2}{12d}\Delta \ln n$ and is not identical to the lattice temperature.

We note that the Bohm potential V_{B} which appears in the QDD$_2$ model is divided by a factor 3 compared with that appearing in the Quantum Hydrodynamic model $\mathcal{V}_{\mathrm{B}}$ (see (5.4)). This factor 3 is not related with the dimension since the derivation has been performed in arbitrary dimension d. The physical reason for this discrepancy between the two models is not yet understood.

We now turn to the QET$_2$ model. It is unfortunate that, in this case, the $\hbar^2$ correction from the CET model does not appear so simple. More precisely, we have:

Theorem 5.2. (i) Let $n^{\hbar}$, $\mathcal{W}^{\hbar}$, $(J^n)^{\hbar}$, $(J^w)^{\hbar}$ be the solution of the Quantum Energy-Transport (QET) model (3.6)–(3.9) with pressure and heat-flux tensors $\Pi^{\hbar}$ and $\mathbb{Q}^{\hbar}$ related with $(n^{\hbar}, \mathcal{W}^{\hbar})$ through (3.4), (3.5) and (3.3). Then, we formally have:

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

where $(n, \mathcal{W}, J^n, J^w)$ satisfies the Quantum Energy-Transport up to order $\hbar^2$ (QET$_2$). The QET$_2$ model consists of the same balance equations (3.6) and (3.7) and constitutive relations (3.8) and (3.9) as the QET model. Only, the relation between the pressure and heat-flux tensors $(\Pi, \mathbb{Q})$ with $(n, \mathcal{W})$ changes and is now given by:

$$\begin{aligned}\Pi_{rs} &= \delta_{rs} n T \\ &\quad + \frac{\hbar^2}{12d} n \delta_{rs} \left(\Delta_x \ln n + 2\Delta_x \ln T + 2\nabla_x \ln n \cdot \nabla_x \ln T - \frac{d+2}{2} |\nabla_x \ln T|^2 \right) \\ &\quad + \frac{\hbar^2}{12} n \left(-\partial^2_{rs} \ln n - 2\partial^2_{rs} \ln T - \partial_r \ln n\, \partial_s \ln T - \partial_r \ln T\, \partial_s \ln n \right. \\ &\qquad \left. + \frac{d+2}{2} \partial_r \ln T\, \partial_s \ln T \right),\end{aligned} \tag{5.11}$$

$$\begin{aligned}\mathbb{Q}_{rs} &= \frac{d+2}{2} \delta_{rs}\, n\, T^2 \\ &\quad + \frac{\hbar^2}{24d} n\, T\, \delta_{rs} \Big((d+4)\Delta_x \ln n + (d+8)\Delta_x \ln T \\ &\quad + 2(d+4)\nabla_x \ln n \cdot \nabla_x \ln T + \frac{d^2-4d-8}{2} |\nabla_x \ln T|^2 \Big) \\ &\quad + \frac{\hbar^2}{24} (d+4)\, n\, T \Big(-\partial^2_{rs} \ln n - 3\partial^2_{rs} \ln T - \partial_r \ln n\, \partial_s \ln T \\ &\qquad - \partial_r \ln T\, \partial_s \ln n + \frac{d}{2} \partial_r \ln T\, \partial_s \ln T \Big),\end{aligned} \tag{5.12}$$

where the generalized temperature T is given by the classical relation

$$T = \frac{2}{d} \frac{\mathcal{W}}{n}. \tag{5.13}$$

We note that there is apparently no entropic structure to the QET$_2$ model. The expansion up to order $\hbar^2$ terms of the entropy $S(n, \mathcal{W})$ defined by (3.10) does not decay along the trajectories of the QET system, or at least, we were unable to prove so.

In order to simplify the QET$_2$ model, we investigate the case where the generalized temperature T varies slowly compared with the density n. To describe this situation, we introduce a small parameter $\eta \ll 1$ and we assume that

$$\frac{|\nabla \ln T|}{|\nabla \ln n|} = \mathcal{O}(\eta).$$

In the limit $\eta \to 0$, we get the following expressions for the currents:

$$\begin{aligned} J^n &= -\nabla\left(n\,T + \frac{\hbar^2}{12d}\,n\,\Delta\ln n\right) - n\,\nabla(V + V_B[n])\,, \\ J^w &= -\nabla\left(\frac{d+2}{2}\,n\,T^2 + \frac{\hbar^2}{24}\,\frac{d+4}{d}\,n\,T\,\Delta\ln n\right) - \frac{d+4}{2}\,n\,T\,\nabla V_B[n] \\ &\quad - \left(\frac{d+2}{2}\,n\,T + \frac{\hbar^2}{12d}\,n\,\Delta\ln n\right)\nabla V + \frac{\hbar^2}{12}\,n\,(\nabla\nabla\ln n)\,\nabla V + \frac{\hbar^2}{8}\nabla\Delta\ln n. \end{aligned}$$

In the next sections, we develop the proofs of theorems 5.1 and 5.2. We first start with some preliminaries.

5.2. Preliminaries

We first prove

Proposition 5.3. Let $a(x, p)$ be a smooth symbol. Then, we have the following expansion:

$$\begin{aligned} \mathcal{E}\mathrm{xp}\; a = \exp a - \frac{\hbar^2}{8}\exp a \Big(& \partial^2_{x_i x_j} a\, \partial^2_{p_i p_j} a - \partial^2_{x_i p_j} a\, \partial^2_{p_i x_j} a + \frac{1}{3}\partial^2_{x_i x_j} a\, \partial_{p_i} a\, \partial_{p_j} a \\ & - \frac{2}{3}\partial^2_{x_i p_j} a\, \partial_{p_i} a\, \partial_{x_j} a + \frac{1}{3}\partial^2_{p_i p_j} a\, \partial_{x_i} a\, \partial_{x_j} a \Big) + \mathcal{O}(\hbar^4), \end{aligned} \qquad (5.14)$$

where Einstein's convention has been used.

First, given two symbols $w_1(x, p)$ and $w_2(x, p)$, we define the operation $w_1 \circ_\hbar w_2$ as the symbol of their operator product, i.e.

$$w_1 \circ_\hbar w_2 = W[W^{-1}(w_1) W^{-1}(w_2)]\,. \qquad (5.15)$$

As a direct application of pseudo-differential calculus (see refs. 1, 45), In ref. 65 we have:

Lemma 5.4. The following formal expansion holds (provided that the symbols w_i are infinitely differentiable):

$$w_1 \circ_{\hbar} w_2(x,p) = \sum_{\alpha,\beta} \left(\frac{i\hbar}{2}\right)^{|\alpha|+|\beta|} \frac{(-1)^{|\beta|}}{\alpha!\beta!} \partial_x^\alpha \partial_p^\beta w_1(x,p)\, \partial_x^\beta \partial_p^\alpha w_2(x,p) \tag{5.16}$$

where $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d$ is a multi-index, $|\alpha| = \sum_i \alpha_i$, $\alpha! = \prod_i \alpha_i!$, $\partial_x^\alpha = \prod_i \partial_{x_i}^{\alpha_i}$ and similarly for β.

Thanks to this Lemma, we can write:

$$w_1 \circ_{\hbar} w_2 = \sum_{n=0}^{\infty} \hbar^n w_1 \circ_n w_2 \tag{5.17}$$

with

$$w_1 \circ_n w_2(x,p) = \sum_{\alpha,\beta,|\alpha|+|\beta|=n} \left(\frac{i}{2}\right)^n \frac{(-1)^{|\beta|}}{\alpha!\beta!} \partial_x^\alpha \partial_p^\beta w_1(x,p)\, \partial_x^\beta \partial_p^\alpha w_2(x,p). \tag{5.18}$$

In particular, we have:

$$w_1 \circ_0 w_2 = w_1 w_2\,, \tag{5.19}$$

$$w_1 \circ_1 w_2 = \frac{i}{2}(\nabla_x w_1 \cdot \nabla_p w_2 - \nabla_p w_1 \cdot \nabla_x w_2) \tag{5.20}$$

$$w_1 \circ_2 w_2 = -\frac{1}{8}(\nabla_x^2 w_1 : \nabla_p^2 w_2 - 2\nabla_x \nabla_p w_1 : \nabla_p \nabla_x w_2 + \nabla_p^2 w_1 : \nabla_x^2 w_2) \tag{5.21}$$

where ∇^2 denotes the Hessian matrix and : the contracted product of tensors. Thanks to the exchange of α and β in (5.18), it is easy to see that

$$w_1 \circ_n w_2 = (-1)^n w_2 \circ_n w_1$$

in other words, the operation $\circ_n$ is commutative (resp. anticommutative) when n is even (resp. odd).

With these preliminaries, we can now prove Proposition 5.3:

Proof of Proposition 5.3. We use the Bloch equation formalism. More precisely, let $F(t) = \mathcal{E}\mathrm{xp}\,(ta) = W[\exp(tW^{-1}(a))]$. Then

$$\begin{aligned}\frac{dF}{dt} &= W[W^{-1}(a)\,\exp(tW^{-1}(a))] = W[\exp(tW^{-1}(a))W^{-1}(a)]\\ &= \frac{1}{2}\{W[W^{-1}(a)\,\exp(tW^{-1}(a))] + W[\exp(tW^{-1}(a))W^{-1}(a)]\}\\ &= \frac{1}{2}(a \circ_{\hbar} F(t) + F(t) \circ_{\hbar} a).\end{aligned}$$

We let $F(0) = 1$, so that $F(1) = W[\exp(W^{-1}(a))] = \mathcal{E}\mathrm{xp}\,(a)$, which is the object to be computed. We expand $F = \sum_{n=0}^{\infty} \hbar^n F_n$.

Then F_n solves:

$$\begin{aligned}\frac{dF_n}{dt} &= \frac{1}{2}\sum_{m=0}^{n} (a \circ_m F_{n-m} + F_{n-m} \circ_m a)\\ &= \sum_{m=0,m\,\mathrm{even}}^{m=n} a \circ_m F_{n-m},\end{aligned}$$

with initial condition $F_n(0) = \delta_{n0}$, where δ_{n0} denotes the Kronecker symbol.

We first have:

$$\frac{dF_0}{dt} = aF_0\,, \quad F_0(0) = 1,$$

which yields $F_0 = e^{at}$. Then, we have:

$$\frac{dF_1}{dt} = aF_1\,, \quad F_1(0) = 0.$$

Thus, $F_1 \equiv 0$. Then:

$$\begin{aligned}\frac{dF_2}{dt} &= a \circ_0 F_2 + a \circ_2 F_0\\ &= aF_2 - \frac{1}{8}(\nabla_x^2 a : \nabla_p^2 F_0 - 2\nabla_x\nabla_p a : \nabla_p\nabla_x F_0 + \nabla_p^2 a : \nabla_x^2 F_0)\\ &= aF_2 - \frac{1}{8}(\nabla_x^2 a : (t\nabla_p^2 a + t^2\nabla_p a\nabla_p a)\\ &\quad -2\nabla_x\nabla_p a : (t\nabla_p\nabla_x a + t^2\nabla_p a\nabla_x a) + \nabla_p^2 a : (t\nabla_x^2 a + t^2\nabla_x a\nabla_x a))F_0\end{aligned}$$

(where the product of two vectors means a tensor product) together with $F_2(0)=0$. Integrating with respect to t, we get:

$$\begin{aligned}F_2(t) = &-\frac{1}{8}(\nabla_x^2 a:(\frac{t^2}{2}\nabla_p^2 a+\frac{t^3}{3}\nabla_p a\nabla_p a)\\ &-2\nabla_x\nabla_p a:(\frac{t^2}{2}\nabla_p\nabla_x a+\frac{t^3}{3}\nabla_p a\nabla_x a)+\nabla_p^2 a:(\frac{t^2}{2}\nabla_x^2 a+\frac{t^3}{3}\nabla_x a\nabla_x a))F_0.\end{aligned}$$

Finally, we have

$$\frac{dF_3}{dt} = a\circ_0 F_3 + a\circ_2 F_1 = aF_3, \quad F_3(0)=0,$$

which gives $F_3\equiv 0$.

We deduce:

$$\begin{aligned}\mathcal{E}\text{xp } a &= e^a\{1-\frac{\hbar^2}{8}[\nabla_x^2 a:(\frac{1}{2}\nabla_p^2 a+\frac{1}{3}\nabla_p a\nabla_p a)\\ &\quad -2\nabla_x\nabla_p a:(\frac{1}{2}\nabla_p\nabla_x a+\frac{1}{3}\nabla_p a\nabla_x a)+\nabla_p^2 a:(\frac{1}{2}\nabla_x^2 a+\frac{1}{3}\nabla_x a\nabla_x a)]\\ &\quad +\mathcal{O}(\hbar^4)\}\\ &= e^a\{1-\frac{\hbar^2}{8}(\nabla_x^2 a:\nabla_p^2 a-\nabla_x\nabla_p a:\nabla_p\nabla_x a\\ &\quad +\frac{1}{3}(\nabla_x^2 a:\nabla_p a\nabla_p a-2\nabla_x\nabla_p a:\nabla_p a\nabla_x a+\nabla_p^2 a:\nabla_x a\nabla_x a))\\ &\quad +\mathcal{O}(\hbar^4)\}, \end{aligned} \tag{5.22}$$

which is formula (5.14) and ends the proof. ▌

We now specialize (5.14) to a symbol of the form: $M(x,p) = \exp(A(x)+C(x)|p|^2)$. Without detailing the computations, we can state:

Lemma 5.5. The following formula holds:

$$\mathcal{E}\text{xp}\left(A(x)+C(x)|p|^2\right) = M-\frac{\hbar^2}{8}M\,F^{(2)}(A,C)+\mathcal{O}(\hbar^4), \tag{5.23}$$

where

$$\begin{aligned}F^{(2)}(A,C) &= 2C\,\partial^2_{ii}A + 2C\,|p|^2\,\partial^2_{ii}C - 4p_ip_j\,\partial_iC\,\partial_jC\\ &\quad+\frac{4}{3}C^2p_ip_j\,\partial^2_{ij}A + \frac{4}{3}C^2p_ip_j\,|p|^2\,\partial^2_{ij}C\\ &\quad-\frac{8}{3}C\,p_ip_j\,\partial_iC\,\partial_jA - \frac{8}{3}C\,p_ip_j\,|p|^2\,\partial_iC\,\partial_jC\\ &\quad+\frac{2}{3}C\,(\partial_iA)^2 + \frac{4}{3}C\,|p|^2\,\partial_iA\,\partial_iC + \frac{2}{3}C\,|p|^4\,(\partial_iC)^2. \qquad (5.24)\end{aligned}$$

For simplicity, $\partial^2_{ij}A$ and $\partial^2_{ij}C$ denote $\partial^2_{x_ix_j}A$ and $\partial^2_{x_ix_j}C$.

At the leading order in $\hbar$, we have $\mathcal{E}\mathrm{xp}\,(A+C|p|^2)=M$. Let us denote

$$\begin{aligned}n_0(t,x) &= \int_{\mathbb{R}^d} M(t,x,p)\,\frac{dp}{(2\pi\hbar)^d} = \int_{\mathbb{R}^d}\exp(A+C|p|^2)\,\frac{dp}{(2\pi\hbar)^d}\\ &= \left(-\frac{\pi}{C}\right)^{d/2}\frac{1}{(2\pi\hbar)^d}\,e^A. \qquad (5.25)\end{aligned}$$

Next, integrating (5.23) with respect to p and using the moments of M computed in Appendix A, we obtain approximations of n, $\mathcal{W}$, Π, $\mathbb{Q}$ (see formulae (3.3)–(3.5)) up to terms of order $\mathcal{O}(\hbar^2)$ as stated in the following:

Lemma 5.6. We have:

$$\begin{aligned}n &= n_0 - \frac{\hbar^2}{6}\,n_0\,C\left(\Delta A + \frac{1}{2}|\nabla A|^2 - \frac{(d-2)}{2}\,\nabla A\cdot\frac{\nabla C}{C}\right.\\ &\qquad\left.-\frac{(d-1)}{2}\,\frac{\Delta C}{C} + \frac{(d^2-2d+4)}{8}\,\frac{|\nabla C|^2}{C^2}\right) + \mathcal{O}(\hbar^4), \qquad (5.26)\\ 2\mathcal{W} &= -\frac{d}{2C}\,n_0 + \frac{\hbar^2}{12}\,n_0\left((d-1)\Delta A + \frac{d}{2}|\nabla A|^2 - \frac{d^2-4}{2}\,\nabla A\cdot\frac{\nabla C}{C}\right.\\ &\qquad\left.-\frac{(d^2-4)}{2}\,\frac{\Delta C}{C} + \frac{(d-2)(d+2)^2}{8}\,\frac{|\nabla C|^2}{C^2}\right), \qquad (5.27)\\ &\qquad (5.28)\end{aligned}$$

and, for any pair r,s of indices:

$$\begin{aligned}\Pi_{rs} = &-\frac{\delta_{rs}}{2C}\,n_0+\frac{\hbar^2}{12}\,n_0\,\delta_{rs}\left(\Delta A+\frac{1}{2}|\nabla A|^2-\frac{d}{2}\,\nabla A\cdot\frac{\nabla C}{C}\right.\\ &\qquad\left.-\frac{(d+1)}{2}\,\frac{\Delta C}{C}+\frac{(d^2+2d+4)}{8}\,\frac{|\nabla C|^2}{C^2}\right)\\ &+\frac{\hbar^2}{12}\,n_0\left(-\partial^2_{rs}A+\partial_r A\,\frac{\partial_s C}{C}+\partial_s A\,\frac{\partial_r C}{C}\right.\\ &\qquad\left.+\frac{(d+4)}{2}\,\frac{\partial^2_{rs}C}{C}-(d+1)\,\frac{\partial_r C\,\partial_s C}{C^2}\right)+\mathcal{O}(\hbar^4)\,,\end{aligned}\tag{5.29}$$

$$\begin{aligned}\mathbb{Q}_{rs} = &\frac{(d+2)\,\delta_{rs}}{8C^2}\,n_0-\frac{\hbar^2}{48}\,\frac{n_0}{C}\,\delta_{rs}\left((d+1)\,\Delta A+\frac{(d+2)}{2}\,|\nabla A|^2\right.\\ &\qquad\left.-\frac{d(d+4)}{2}\,\nabla A\cdot\frac{\nabla C}{C}-\frac{d(d+4)}{2}\,\frac{\Delta C}{C}+\frac{d(d+4)^2}{8}\,\frac{|\nabla C|^2}{C^2}\right)\\ &-\frac{\hbar^2}{48}\,\frac{n_0}{C}\left(-(d+4)\,\partial^2_{rs}A+(d+4)\,\partial_r A\,\frac{\partial_s C}{C}+(d+4)\,\partial_s A\,\frac{\partial_r C}{C}\right.\\ &\qquad\left.+\frac{(d+4)(d+6)}{2}\,\frac{\partial^2_{rs}C}{C}-(d+3)(d+4)\,\frac{\partial_r C\,\partial_s C}{C^2}\right)+\mathcal{O}(\hbar^4)\,.\end{aligned}\tag{5.30}$$

We note that (5.27) can be deduced from (5.29) because $2\mathcal{W}=\operatorname{Tr}\Pi$.

After these preliminaries, we can proceed to the proof of Theorem 5.1.

5.3. Proof of Theorem 5.1

(i) In the case of the Quantum Drift-Diffusion, the temperature T_0 is specified and we have $C=-1/(2T_0)$. Therefore (5.25), (5.26) and (5.29) become

$$n_0=\left(\frac{2\pi T_0}{(2\pi\hbar)^2}\right)^{d/2}\,e^A,\tag{5.31}$$

$$n=n_0+\frac{\hbar^2}{12}\,\frac{n}{T_0}\left(\Delta A+\frac{1}{2}\,|\nabla A|^2\right)+\mathcal{O}(\hbar^4),\tag{5.32}$$

$$\begin{aligned}\Pi_{rs}&=\delta_{rs}\,T_0\,n_0+\frac{\hbar^2}{12}\,n_0\left(\delta_{rs}\,\Delta A+\frac{1}{2}\,\delta_{rs}\,|\nabla A|^2-\,\partial^2_{rs}A\right)+\mathcal{O}(\hbar^4)\\ &=\delta_{rs}\,T_0\,n-\frac{\hbar^2}{12}\,n\,\partial^2_{rs}A+\mathcal{O}(\hbar^4).\end{aligned}\tag{5.33}$$

Eq. (5.33) relates Π to n and A. But A is related with n through (5.31) and (5.32). We want to use these relations to eliminate A from (5.33), or, more precisely, from the term $-\nabla\cdot\Pi$ which appears in the current equation (4.10). In the course of this computation, we are allowed to drop terms of order $\hbar^4$ or more. Thanks to (5.33), we have

$$-(\nabla\cdot\Pi)_r = -\sum_s \partial_s \Pi_{rs} = -T_0\,\partial_r n + \frac{\hbar^2}{12}\left(\sum_s \partial_s n\,\partial^2_{rs}A + n\sum_s \partial^3_{rss}A\right) + \mathcal{O}(\hbar^4).$$

But, from (5.31), we have:

$$\ln n_0 = A + \frac{d}{2}\ln(2\pi T_0) - d\ln(2\pi\hbar) = A - K_{T_0},$$

thus defining the constant K_{T_0}. Hence we deduce that

$$\nabla A = \frac{\nabla n_0}{n_0} = \frac{\nabla n}{n} + \mathcal{O}(\hbar^2)$$

and consequently, that

$$-\nabla\cdot\Pi = -T_0\nabla n + \frac{\hbar^2}{12}\,n\,\nabla\left(\Delta A + \frac{1}{2}|\nabla A|^2\right) + \mathcal{O}(\hbar^4)\,.$$

Besides, the identity

$$\Delta A = \frac{\Delta n}{n} - \frac{|\nabla n|^2}{n^2} + \mathcal{O}(\hbar^2),$$

implies that

$$\Delta A + \frac{1}{2}|\nabla A|^2 = \frac{\Delta n}{n} - \frac{1}{2}\,\frac{|\nabla n|^2}{n^2} + \mathcal{O}(\hbar^2) = 2\frac{\Delta\sqrt{n}}{\sqrt{n}} + \mathcal{O}(\hbar^2).$$

Therefore, if we introduce the quantum Bohm potential $V_B[n]$ according to (5.7), we get

$$-\nabla\cdot\Pi = -T_0\,\nabla n - n\,\nabla V_{\mathrm{B}}[n] + \mathcal{O}(\hbar^4). \qquad (5.34)$$

Inserting this expansion in (4.10) and omitting the remainder of order $\mathcal{O}(\hbar^4)$, we get (5.6), which ends the proof of part (i) of the theorem.

(ii) We now recall that the fluid entropy introduced in Section 4 is

$$\widetilde{S}[n]=\int_{\mathbb{R}^d} n\left(A+\frac{V}{T_0}-1\right)dx.$$

Let us expand this expression with respect to $\hbar$. We have $A=\ln n_0+K_{T_0}$. Moreover (5.32) gives

$$\ln n_0=\ln n-\frac{\hbar^2}{12}\frac{1}{T_0}\left(\Delta A+\frac{1}{2}|\nabla A|^2\right)+\mathcal{O}(\hbar^4),$$

from which we deduce:

$$\begin{aligned}
&n\left(A+\frac{V}{T}-1\right)=\\
&=n\left(\ln n-\frac{\hbar^2}{12}\frac{1}{T_0}\left(\Delta A+\frac{1}{2}|\nabla A|^2\right)+K_{T_0}+\frac{V}{T_0}-1\right)+\mathcal{O}(\hbar^4)\\
&=n\left(\ln n+\frac{V_B[n]}{T_0}+K_{T_0}+\frac{V}{T_0}-1\right)+\mathcal{O}(\hbar^4).
\end{aligned}$$

Consequently we obtain

$$\widetilde{S}[n]=\int_{\mathbb{R}^d} n\left(\ln n-1+\frac{V+V_B[n]}{T_0}+K_{T_0}\right)dx+\mathcal{O}(\hbar^4).$$

We note that, since $\int n\,dx$ is a constant, the term $\int nK_{T_0}\,dx$ is a constant and can therefore be removed from the definition of the entropy. Therefore, the fluid entropy at the order $\hbar^2$, $\widetilde{S}_2[n]$ can be defined according to (5.8).

Furthermore, straightforward computations show that, for non-negative functions n, $\widetilde{S}_2[n]$ is a twice Gâteaux differentiable convex functional. Its first and second derivatives evaluated at n in the direction δn are given by:

$$D\widetilde{S}_2[n](\delta n)=\int_{\mathbb{R}^d}\left(\ln n+\frac{V+V_{\mathrm{B}}[n]}{T_0}\right)\delta n\,dx\,, \tag{5.35}$$

and

$$D^2\widetilde{S}_2[n](\delta n,\delta n)=\int_{\mathbb{R}^d}\frac{1}{n}\left((\delta n)^2+\frac{\hbar^2}{12T_0}\left|\nabla\delta n-\delta n\frac{\nabla n}{n}\right|^2\right)dx. \tag{5.36}$$

Now, suppose that n is a solution of the QDD_2 model (5.5), (5.6). From (5.35) we deduce that

$$\begin{aligned}\frac{d}{dt}\widetilde{S}_2[n] &= D\widetilde{S}_2[n](\partial_t n) + \int_{\mathbb{R}^d} n\frac{\partial_t V}{T_0}\,dx \\ &= \frac{1}{T_0}\int_{\mathbb{R}^d}(T_0 \ln n + V + V_B[n])\,\partial_t n\,dx + \int_{\mathbb{R}^d} n\frac{\partial_t V}{T_0}\,dx. \qquad (5.37)\end{aligned}$$

Then, using (5.5) and (5.6), we get:

$$\begin{aligned}\frac{d}{dt}\widetilde{S}_2(n) = \frac{1}{T_0}\int_{\mathbb{R}^d}(T_0 \ln n + V + V_B[n])\,\nabla\cdot(T_0\,\nabla n + n\,\nabla(V + V_B[n]))\,dx \\ + \int_{\mathbb{R}^d} n\frac{\partial_t V}{T_0}\,dx.\end{aligned}$$

Formula (5.9) follows after applying Green's formula. ▮

5.4. Proof of Theorem 5.2

We want to perform the same kind of manipulations as in the proof of Theorem 5.1, in order to pass from (5.29), (5.30) to (5.11), (5.13). For that purpose, we need to eliminate A and C from (5.29), (5.30) in favour of n and $\mathcal{W}$ (or equivalently, in favour of T given by (5.13)).

For convenience, we define $T_0 = -1/(2C)$. This quantity T_0 is the temperature of the system (not equal to the generalized temperature T defined by (5.13)). From (5.25), (5.26) and (5.29), we deduce the following relations:

$$\begin{aligned}&n = n_0 + \mathcal{O}(h^2), \qquad T = T_0 + \mathcal{O}(h^2), \qquad \frac{\nabla C}{C} = -\nabla \ln T + \mathcal{O}(h^2), \\ &A = \ln n - \frac{d}{2}\ln T + \frac{d}{2}\ln(2\pi\hbar^2) + \mathcal{O}(h^2).\end{aligned}$$

Then by straightforward calculations from (5.26) and (5.27), we obtain

$$\begin{aligned}n &= n_0 + \frac{\hbar^2}{12}\frac{n}{T}\left(\Delta \ln n + \frac{1}{2}|\nabla \ln n|^2 - \nabla \ln n\cdot\nabla \ln T \right. \\ &\qquad \left. -\frac{1}{2}\Delta \ln T - \frac{(d-4)}{4}|\nabla \ln T|^2\right) + \mathcal{O}(h^4), \qquad (5.38) \\ n\,T &= n_0\,T_0 + \frac{\hbar^2}{12d}\,n\left((d-1)\Delta \ln n + \frac{d}{2}|\nabla \ln n|^2 - 2\nabla \ln n\cdot\nabla \ln T \right. \\ &\qquad \left. + \frac{d-4}{2}\Delta \ln T - \frac{d^2-2d-4}{4}|\nabla \ln\,T|^2\right) + \mathcal{O}(h^4). \qquad (5.39)\end{aligned}$$

Inserting these relations into (5.29) and (5.30) and keeping the leading order terms, we find (5.11) and (5.13). ▮

6. CONCLUSION

In this paper, we have proposed new Quantum Energy-Transport and Quantum Drift-Diffusion models. These models are derived from a diffusion limit of a collisional Wigner equation. We have used simplified relaxation collision operators but which retain some important quantum features: quantum entropy decay and relaxation towards quantum equilibria. The resulting models involve fluxes which are related in a non-local way to the state variables. Nonetheless, these models are consistant with quantum entropy decay. An expansion in powers of $\hbar$ allows to simplify these relations. Keeping the leading order quantum correction in the Drift-Diffusion model amounts to adding the Bohm potential to the classical model. We can prove that this model is still entropic. The leading order quantum correction to the Energy-Transport model is unfortunately not so simple. Future developments of this work will involve both theoretical investigations (proof of well-posedness, stability, etc.), and numerical ones.

7. Appendix A

In order to expand the different moments of $\mathcal{E}\mathrm{xp}\,(A + C|p|^2)$, we need to compute the moments of $M = \exp(A + C|p|^2)$ in terms of $n_0 = \int_{\mathbb{R}^d} M \frac{dp}{(2\pi\hbar)^d}$. In the following formulae, the indices r, s, i, j, k and l are given and $\delta_{\alpha_1\alpha_2\ldots\alpha_n}$ is a generalization of the Kronecker symbol for n indices):

$$\int_{\mathbb{R}^d} p_i\, p_j\, M \frac{dp}{(2\pi\hbar)^d} = -\frac{n_0}{2C}\,\delta_{ij},$$

$$\int_{\mathbb{R}^d} p_r\, p_s\, p_i\, p_j\, M \frac{dp}{(2\pi\hbar)^d} = \frac{n_0}{4C^2}\,(\delta_{rs}\,\delta_{ij} + \delta_{ri}\,\delta_{sj} + \delta_{rj}\,\delta_{si}),$$

$$\int_{\mathbb{R}^d} p_i\, p_j\, |p_k|^2\, M \frac{dp}{(2\pi\hbar)^d} = \frac{n_0}{4C^2}\,\delta_{ij}\,(2\delta_{ik} + 1),$$

$$\begin{aligned}\int_{\mathbb{R}^d} & p_r\, p_s\, p_i\, p_j\, |p_k|^2\, M \frac{dp}{(2\pi\hbar)^d} \\ &= -\frac{n_0}{8C^3}\,(\delta_{rs}\,\delta_{ij} + \delta_{ri}\,\delta_{sj} + \delta_{rj}\,\delta_{si} \\ &\quad + 2\delta_{rsk}\,\delta_{ij} + 2\delta_{rs}\,\delta_{ijk} + 2\delta_{rik}\,\delta_{sj} + 2\delta_{ri}\,\delta_{sjk} \\ &\quad + 2\delta_{rjk}\,\delta_{si} + 2\delta_{rj}\,\delta_{sik}),\end{aligned}$$

$$\begin{aligned}
&\int_{\mathbb{R}^d} p_r\, p_s\, p_i\, p_j\, |p_k|^2\, |p_l|^2\, M\, \frac{dp}{(2\pi\hbar)^d}\\
&\quad = \frac{n_0}{16C^4}\,(\delta_{rs}\,\delta_{ij} + \delta_{ri}\,\delta_{sj} + \delta_{rj}\,\delta_{si}\\
&\qquad +2\delta_{rs}\,\delta_{ij}\,\delta_{kl} + 2\delta_{ri}\,\delta_{sj}\,\delta_{kl} + 2\delta_{rj}\,\delta_{si}\,\delta_{kl}\\
&\qquad +2\delta_{rsk}\,\delta_{ij} + 2\delta_{rs}\,\delta_{ijk} + 2\delta_{rik}\,\delta_{sj} + 2\delta_{ri}\,\delta_{sjk} + 2\delta_{rjk}\,\delta_{si} + 2\delta_{rj}\,\delta_{sik}\\
&\qquad +2\delta_{rsl}\,\delta_{ij} + 2\delta_{rs}\,\delta_{ijl} + 2\delta_{ril}\,\delta_{sj} + 2\delta_{ri}\,\delta_{sjl} + 2\delta_{rjl}\,\delta_{si} + 2\delta_{rj}\,\delta_{sil}\\
&\qquad +4\delta_{rsk}\,\delta_{ijl} + 4\delta_{rsl}\,\delta_{ijk} + 4\delta_{rik}\,\delta_{sjl} + 4\delta_{ril}\,\delta_{sjk} + 4\delta_{rjk}\,\delta_{sil} + 4\delta_{rjl}\,\delta_{sik}\\
&\qquad +8\delta_{rskl}\,\delta_{ij} + 8\delta_{rs}\,\delta_{ijkl} + 8\delta_{rikl}\,\delta_{sj} + 8\delta_{ri}\,\delta_{sjkl} + 8\delta_{rjkl}\,\delta_{si} + 8\delta_{rj}\,\delta_{sikl}).
\end{aligned}$$

Hence after some summations, for any (r, s, i, j), we deduce

$$\begin{aligned}
&\int_{\mathbb{R}^d} |p|^2 M \frac{dp}{(2\pi\hbar)^d} = -\frac{n_0}{2C}d,\\
&\int_{\mathbb{R}^d} p_i\, p_j\, |p|^2 M \frac{dp}{(2\pi\hbar)^d} = \frac{n_0}{4C^2}\delta_{ij}\,(d+2),\\
&\int_{\mathbb{R}^d} |p|^4 M \frac{dp}{(2\pi\hbar)^d} = \frac{n_0}{4C^2}d(d+2),\\
&\int_{\mathbb{R}^d} p_r\, p_s\, p_i\, p_j\, |p|^2 M \frac{dp}{(2\pi\hbar)^d} = -\frac{n_0}{8C^3}(\delta_{rs}\delta_{ij} + \delta_{ri}\delta_{sj} + \delta_{rj}\delta_{si})(d+4),\\
&\int_{\mathbb{R}^d} p_r\, p_s\, |p|^4 M \frac{dp}{(2\pi\hbar)^d} = -\frac{n_0}{8C^3}\delta_{rs}\,(d+2)(d+4),\\
&\int_{\mathbb{R}^d} p_r\, p_s\, p_i\, p_j\, |p|^4 M \frac{dp}{(2\pi\hbar)^d} = \frac{n_0}{16C^4}(\delta_{rs}\delta_{ij} + \delta_{ri}\delta_{sj} + \delta_{rj}\delta_{si})(d+4)(d+6),\\
&\int_{\mathbb{R}^d} p_r\, p_s\, |p|^6 M \frac{dp}{(2\pi\hbar)^d} = \frac{n_0}{16C^4}\delta_{rs}\,(d+2)(d+4)(d+6).
\end{aligned}$$

ACKNOWLEDGMENT

Supported by the European network HYKE, funded by the EC as contract HPRN-CT-2002-00282, and by NSF grant DECS-0218008.

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