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# Quantum hydrodynamic and diffusion models derived from the entropy principle

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**Summary.** In these notes, we review the recent theory of quantum hydrodynamic and diffusion models derived from the entropy minimization principle. These models are obtained by taking the moments of a collisional Wigner equation and closing the resulting system of equations by a quantum equilibrium. Such an equilibrium is defined as a minimizer of the quantum entropy subject to local constraints of given moments. We provide a framework to develop this minimization approach and successively apply it to quantum hydrodynamic models and quantum diffusion models. The results of numerical simulations show that these models capture well the various features of quantum transport.

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## 1 General introduction

The goal of these lecture notes is to give a comprehensive introduction to the theory of quantum hydrodynamic and diffusion models derived from the entropy principle. These lecture notes report on previously published works [25, 26, 23, 24, 21, 22].

These models are obtained by taking the moments of a collisional Wigner equation and closing the resulting system of equations by a quantum equilibrium. Such an equilibrium is defined as a minimizer of the quantum entropy subject to local constraints of given moments. We provide a framework to develop this minimization approach and successively apply it to quantum hydrodynamic models and quantum diffusion models. We also give some preliminary numerical results.

These lecture notes are organized as follows. In section 2 and particularly in sub-section 2.1, an introduction to quantum kinetic theory is given. Sub-section 2.2 is devoted to a presentation of the  $N$ -particle problem in quantum mechanics and the Hartree and Hartree-Fock approximations. With these notions in hand, it is possible to give a very short and incomplete summary of methods that are in use for modeling large quantum particle systems in sub-section 2.3. Current quantum hydrodynamic approaches are then introduced in sub-section 2.4.

Section 3 tackles the core of the matter, the derivation of quantum hydrodynamic models based on the entropy principle. The setting of the problem is recalled in sub-section 3.1. Then, general quantum hydrodynamic models are derived in sub-section 3.2. Finally, a detailed analysis of the isothermal quantum Euler model is developed in sub-section 3.3, and illustrated by some preliminary numerical simulations.

Section 4 turns towards quantum diffusion models. First, the quantum Energy-Transport model is developed in sub-section 4.1. The case of the quantum drift-diffusion model is reviewed in sub-section 4.2. In the latter case, detailed numerical simulations are given which show that the model captures well the various features of diffusive quantum transport.

Finally, conclusions and perspectives are drawn in section 5.

## 2 Quantum kinetic equations: an introduction

### 2.1 Quantum statistical mechanics of nonequilibrium systems

In quantum mechanics, the state of a particle is defined by a wave-function  $\psi(x, t) \in \mathbb{C}$ , where  $x \in \mathbb{R}^d$  is the position and  $t$  the time. The quantity  $dP_t(x) = |\psi(x, t)|^2 dx$  represents the probability of finding the particle in the elementary volume  $dx$  at time  $t$ . As such, we have the normalization condition

$$\int |\psi(x, t)|^2 dx = \int dP_t(x) = 1. \quad (1)$$

Therefore,  $\psi(\cdot, t) \in L^2(\mathbb{R}^d)$ . We denote by  $d$  the dimension of configuration space. The evolution of  $\psi$  is ruled by the Schrödinger equation

$$i\hbar\partial_t\psi = \mathcal{H}\psi, \quad (2)$$

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

$$\mathcal{H}\psi = -\frac{\hbar^2}{2}\Delta\psi + V(x, t)\psi, \quad (3)$$

where  $V(x, t)$  is the potential energy.

A measurement of the system gives rise to the operation

$$(\psi, A\psi)_{L^2} = \int \psi \overline{A\psi} dx, \quad (4)$$

where  $A$  is a Hermitian operator on  $L^2$  which corresponds to the physical quantity to be measured and the bar denotes complex conjugation. For instance, the position operator  $X : \psi \rightarrow x\psi(x)$  corresponds to the observation of the mean particle position:

$$(\psi, X\psi) = \int x |\psi|^2 dx.$$

Similarly, the momentum operator  $P : \psi \rightarrow -i\hbar\nabla\psi$  gives rise to the observation

$$(\psi, P\psi) = -\int \psi \overline{i\hbar\nabla\psi} dx = \int \hbar k |\hat{\psi}(k)|^2 dk,$$

where  $\hat{\psi}(k)$  is Fourier transform of  $\psi$ :

$$\hat{\psi}(k) = (2\pi)^{-d/2} \int e^{-ik \cdot x} \psi(x) dx.$$

Any classical observable  $a(x, p)$  gives rise to a quantum observable  $A = \text{Op}(a)$  according to the Weyl quantization rule:

$$\text{Op}(a)\psi = \frac{1}{(2\pi)^d} \int a\left(\frac{x+y}{2}, \hbar k\right) \psi(y) e^{ik(x-y)} dk dy, \quad (5)$$

and  $a$  is called the Weyl symbol of  $\text{Op}(a)$ . An example of such observable is the mechanical energy or Hamiltonian  $\mathcal{H}_c(x, p) = |p|^2/2 + V$  which gives rise to the quantum Hamiltonian operator

$$\text{Op}(\mathcal{H}_c) = \mathcal{H} = -(\hbar^2/2)\Delta + V. \quad (6)$$

For an N-particle systems, the wave-function  $\psi(x_1, \dots, x_N)$  depends on all the coordinates of the N particles: here,  $x_i$  denotes the coordinate of the i-th particle. In this case, the classical Hamiltonian is written

$$\mathcal{H}_c = \sum_{i=1}^N \frac{1}{2}|p_i|^2 + \frac{1}{2} \sum_{i \neq j} \phi_{int}(x_i - x_j) + \sum_i \phi_{ext}(x_i), \quad (7)$$

with  $\phi_{int}(x - y)$  a binary interaction potential and  $\phi_{ext}(x)$  an external potential. Its quantum counterpart is:

$$\mathcal{H} = - \sum_{i=1}^N \frac{\hbar^2}{2} \Delta_{x_i} + \frac{1}{2} \sum_{i \neq j} \phi_{int}(x_i - x_j) + \sum_i \phi_{ext}(x_i). \quad (8)$$

When the state of an N-particle system is incompletely known, a statistical description is needed. To describe the uncertainty about the state of the system we make use of a complete orthonormal basis of the system  $(\phi_s)_{s \in S}$  and  $\rho_s$  lists the occupation probability of state  $s$  i.e. the probability that a particle lies in the state  $s$ . Being probabilities,  $\rho_s$  satisfies

$$0 \leq \rho_s \leq 1, \quad \sum_{s \in S} \rho_s = 1. \quad (9)$$

The probability of presence of a particle in the incompletely known system described by the set  $(\rho_s)_{s \in S}$  is given by:

$$P(x, t) dx = \sum_{s \in S} \rho_s |\phi_s|^2 dx. \quad (10)$$

To compute the evolution of an incompletely known system, it is necessary to make a bookkeeping of the states  $(\phi_s)_{s \in S}$  and the probabilities  $(\rho_s)_{s \in S}$ . In order to do so, one introduces an operator on  $L^2$ , the so-called density operator  $\rho$ , defined by its action on an arbitrary  $\psi \in L^2$  by:

$$\rho\psi = \sum_{s \in S} \rho_s (\psi, \phi_s) \phi_s. \quad (11)$$

This defines  $\rho$  as an Hermitian, positive operator whose eigenvectors are  $\phi_s$  and eigenvalues  $\rho_s$ . Then, because of (9),  $\rho$  is trace-class and its trace is unity:

$$\text{Tr } \rho = \sum_{s \in S} \rho_s = 1. \quad (12)$$

Such an incompletely known system is said to be in a mixed state. The case of a pure state is when all  $\rho_s$  are zero but one, say  $\rho_{s_0} = 1$ . Then  $\rho = (\cdot, \phi_{s_0}) \phi_{s_0}$  is nothing but the projection on the one-dimensional manifold spanned by  $\phi_{s_0}$ .

Now, to compute the evolution of  $\rho$  we suppose that  $\phi_s(t)$  is a solution of Schrödinger equation for all  $s$  and that the probabilities  $\rho_s$  do not evolve with time:  $\rho_s(t) = \text{constant}$ . Then, the equation for  $\rho$  reads

$$i\hbar \partial_t \rho = \mathcal{H}\rho - \rho\mathcal{H} = [\mathcal{H}, \rho], \quad (13)$$

and is called the Quantum Liouville equation. From now on  $[\mathcal{A}, \mathcal{B}]$  will denote the commutator of operators  $\mathcal{A}$  and  $\mathcal{B}$ , i.e.  $[\mathcal{A}, \mathcal{B}] = \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A}$ .

Another way of defining  $\rho$  is through its distribution kernel  $\underline{\rho}(x, x')$  defined by

$$\rho\psi = \int \underline{\rho}(x, x') \psi(x') dx'. \quad (14)$$

With (11), we have

$$\underline{\rho}(x, x') = \sum_s \rho_s \phi_s(x) \overline{\phi_s(x')}. \quad (15)$$

The Quantum Liouville equation expressed in terms of  $\underline{\rho}(x, x')$  is written

$$i\hbar \partial_t \underline{\rho} = (\mathcal{H}_x - \mathcal{H}_{x'}) \underline{\rho}, \quad (16)$$

where  $\mathcal{H}_x$  (resp.  $\mathcal{H}_{x'}$ ) denotes the Hamiltonian applied to the  $x$  (resp.  $x'$ ) dependence of  $\underline{\rho}(x, x')$ . We note that, because  $\rho$  is Hermitian,

$$\underline{\rho}(x', x) = \overline{\underline{\rho}(x, x')}, \quad (17)$$

and that its trace is given by

$$\text{Tr} \rho = \int \underline{\rho}(x, x) dx. \quad (18)$$

Now, we turn to the observation of a statistical quantum system defined by its density operator  $\rho$ . Let  $A$  be an observable. Then, the observation of the system is

$$\langle A \rangle_\rho = \sum_s \rho_s \langle A \phi_s, \phi_s \rangle = \text{Tr}\{\rho A\}. \quad (19)$$

For example the probability of presence at  $x_0$  is given by

$$\begin{aligned} P(x_0) &= \sum_{s \in S} \rho_s |\phi_s(x_0)|^2 \\ &= \underline{\rho}(x_0, x_0) = \text{Tr}\{\rho \text{Op}(\delta_{x-x_0})\}, \end{aligned} \quad (20)$$

and is the observation of the state at  $x = x_0$ .

The Wigner transform of  $\rho$  allows to write the observation associated with observable  $A$  in terms of its Weyl symbol  $A = \text{Op}(a)$ , according to the following formula:

$$\begin{aligned} \langle \text{Op}(a) \rangle_\rho &= \text{Tr}\{\rho \text{Op}(a)\} \\ &= \frac{1}{(2\pi\hbar)^d} \int W[\rho](x, p) a(x, p) dx dp, \end{aligned} \quad (21)$$

and  $W[\rho]$  is the so-called Wigner transform of  $\rho$ . In other words,

$$W[\rho](x_0, p_0) = (2\pi\hbar)^d \langle \text{Op}(\delta_{x-x_0} \delta_{p-p_0}) \rangle_\rho, \quad (22)$$

is up to the factor  $(2\pi\hbar)^d$ , the observation of the system at  $(x_0, p_0)$ .

For such a formula to be valid,  $W[\rho]$  must be defined by

$$W[\rho](x, p) = \int \underline{\rho}\left(x - \frac{\eta}{2}, x + \frac{\eta}{2}\right) e^{\frac{i\eta \cdot p}{\hbar}} d\eta, \quad (23)$$

and, with  $\underline{\rho}$  defined by (15), we find

$$W[\rho](x, p) = \sum_s \rho_s \int \phi_s(x - \frac{\eta}{2}) \overline{\phi_s(x + \frac{\eta}{2})} e^{\frac{i\eta \cdot p}{\hbar}} d\eta. \quad (24)$$

Note that  $W[\rho]$  is real-valued (thanks to (17)) but is not necessary positive. Therefore,  $W[\rho] dx dp$  is not a probability distribution function (as would a classical distribution function be). However, the Husimi regularization, defined by

$$W_H[\rho] = W[\rho] * G, \quad G = \frac{1}{(\hbar\pi)^3} e^{-(|x|^2 + |p|^2)/\hbar},$$

is actually non negative.

Applying the Wigner transform to the Quantum Liouville eq. for  $\rho$  (13), we find the Wigner equation for  $W[\rho]$ :

$$\partial_t W + p \cdot \nabla_x W + \Theta^{\hbar}[V]W = 0, \quad (25)$$

where the field operator  $\Theta^{\hbar}[V]W$  is defined by:

$$\begin{aligned} \Theta^{\hbar}[V]W = & -\frac{i}{(2\pi)^3 \hbar} \int (V(x + \frac{\hbar}{2}\eta) - V(x - \frac{\hbar}{2}\eta)) \times \\ & \times W(x, q) e^{i\eta \cdot (p - q)} dq d\eta. \end{aligned} \quad (26)$$

The Wigner equation resembles the classical collisionless kinetic equation (or Vlasov equation) but for the field term  $\Theta^{\hbar}[V]$ . However, as the Planck constant  $\hbar$  tends to zero, we have

$$\Theta^{\hbar}[V]W \xrightarrow{\hbar \rightarrow 0} -\nabla_x V \cdot \nabla_p W. \quad (27)$$

Using the Parseval identity, we have

$$\int W[\rho] \overline{W[\sigma]} \frac{dx dp}{(2\pi\hbar)^d} = \text{Tr}\{\rho \sigma^\dagger\}, \quad (28)$$

$$\int a \bar{b} \frac{dx dp}{(2\pi\hbar)^d} = \text{Tr}\{\text{Op}(a) \text{Op}(b)^\dagger\}, \quad (29)$$

where the superscript  $\dagger$  indicates the Hermitian conjugate operator. The Wigner transformation and the Weyl quantization are inverse operations one to each other and are isometries between the space of  $L^2(\mathbb{R}^{2d})$  functions of  $(x, p)$  (equipped with the measure  $(2\pi\hbar)^{-d} dx dp$ ) and the space  $\mathcal{L}^2$  of operators  $\sigma$  on  $L^2(\mathbb{R}^d)$  such that the product  $\sigma\sigma^\dagger$  is trace class (equipped with the norm  $|\sigma|_{\mathcal{L}^2}^2 = \text{Tr}\{\sigma\sigma^\dagger\}$ ):

$$W = \text{Op}^{-1}, \quad \text{Op} = W^{-1}.$$

Note that elements of the space  $\mathcal{L}^2$  are the so-called Hilbert-Schmidt operators.

## 2.2 N-particle quantum system

In this section, we review some of the standard techniques to deal with many-particle quantum systems, namely the Hartree and the Hartree-Fock methods.

For an N-particle quantum system, the density operator is an operator  $\rho^N$  operating on  $L^2(\mathbb{R}^{3N})$  whose distribution kernel is  $\underline{\rho}^N(x_1, x'_1, \dots, x_N, x'_N)$ . Now, we have to enforce the undistinguishability of the particles, which translates to the fact that the density operator is invariant under permutations of the particles:

$$\underline{\rho}^N(x_{\sigma(1)}, x'_{\sigma(1)}, \dots, x_{\sigma(N)}, x'_{\sigma(N)}) = \underline{\rho}^N(x_1, x'_1, \dots, x_N, x'_N), \quad (30)$$

for all permutations  $\sigma$  of the set  $\{1, 2, \dots, N\}$ . The Quantum Liouville equation is written

$$i\hbar\partial_t\rho^N = [\mathcal{H}^N, \rho^N], \quad (31)$$

$$\mathcal{H}^N = \sum_{i=1}^N \frac{1}{2}|p_i|^2 + \frac{1}{2} \sum_{i \neq j} \phi(x_i - x_j), \quad (32)$$

where  $\phi$  describes the potential for binary interactions between the particles.

We now define partial density operators by taking the partial trace with respect to the last  $N - j$  variables, i.e.

$$\rho^j = \text{Tr}_{j+1}^N\{\rho^N\}, \quad (33)$$

$$\begin{aligned} \underline{\rho}^j(x_1, x'_1, \dots, x_j, x'_j) &= \\ &= \int \underline{\rho}^N(\dots, x_{j+1}, x_{j+1}, \dots, x_N, x_N) dx_{j+1} \dots dx_N. \end{aligned} \quad (34)$$

Taking the partial trace of the quantum Liouville equation over the last  $N - j$  variables, we find the equation satisfied by  $\rho^j$

$$i\hbar\partial_t\rho^j = [\mathcal{H}^j, \rho^j] + Q^j(\rho^{j+1}), \quad (35)$$

$$\mathcal{H}^j = \sum_{i=1}^j \frac{1}{2}|p_i|^2 + \frac{1}{2} \sum_{i,k=1, i \neq k}^j \phi(x_i - x_k). \quad (36)$$

The equation for  $\rho^j$  depends on  $\rho^{j+1}$  and so on up to  $\rho^N$ . This forms a hierarchy of equations called the quantum BBGKY hierarchy, after the works of Bogoliubov, Born, Green, Kirkwood and Yvon. The interaction operator is written,

$$Q^j(\rho^{j+1}) = (N - j) \sum_{i=1}^j \text{Tr}_{j+1}\{\phi(x_i - x_{j+1}), \rho^{j+1}\}. \quad (37)$$

The invariance of  $\rho^N$  under permutations allows to have only the variable  $x_{j+1}$  coming into this expression instead of the whole list  $x_{j+1}, \dots, x_N$ . In particular, the equation for  $\rho^1$  is given by

$$i\hbar\partial_t\rho^1 = [\mathcal{H}^1, \rho^1] + Q^1(\rho^2), \quad (38)$$

$$\mathcal{H}^1 = \frac{1}{2}|p_1|^2, \quad (39)$$

$$Q^1(\rho^2) = (N-1)\text{Tr}_2\{[\phi(x_1 - x_2), \rho^2]\}, \quad (40)$$

or,

$$\underline{Q}^1(\rho^2) = (N-1) \int [\phi(x_1 - x_2) - \phi(x'_1 - x_2)] \underline{\rho}^2(x_1, x'_1, x_2, x_2) dx_2. \quad (41)$$

The goal is to find a closed system for  $\rho^1$  only. For that purpose, we need to find a prescription for  $\rho^2$ . The most simple one is that of statistical independence, also called propagation of chaos, which states that  $\rho^2$  is a product of a one-particle density:

$$\underline{\rho}^2(x_1, x'_1, x_2, x'_2) = \underline{\rho}^1(x_1, x'_1) \underline{\rho}^1(x_2, x'_2). \quad (42)$$

The choice can be rigorously justified in the limit  $N \rightarrow \infty$ , provided that a rescaling of the interaction strength between the particles is made, namely rescaling  $\phi$  into  $\frac{1}{N}\phi$ . The rationale of this rescaling is keeping the force acting on a single particle finite, which allows to capture the limiting dynamics as  $N \rightarrow \infty$  without any time rescaling.

Using (42), we find

$$\begin{aligned} \underline{Q}^1(\rho^2) &= (1 - (1/N)) \int [\phi(x_1 - x_2) - \phi(x'_1 - x_2)] \underline{\rho}^2(x_1, x'_1, x_2, x_2) dx_2 \\ &\approx \int [\phi(x_1 - x_2) - \phi(x'_1 - x_2)] \underline{\rho}^1(x_2, x_2) dx_2 \underline{\rho}^1(x_1, x'_1). \end{aligned} \quad (43)$$

We can write

$$\underline{Q}^1(\rho^2) \approx (V_\rho(x_1) - V_\rho(x'_1)) \underline{\rho}^1(x_1, x'_1), \quad (44)$$

or

$$Q^1(\rho^2) \approx [V_\rho, \rho^1] \quad (45)$$

with

$$V_\rho(x) = \int \phi(x - y) \underline{\rho}^1(y, y) dy. \quad (46)$$

Finally, we find the density operator formulation of Schrödinger mean-field equations:

$$i\hbar\partial_t\rho = [\mathcal{H}_{mf}, \rho], \quad (47)$$

$$\mathcal{H}_{mf} = \frac{1}{2}|p|^2 + V_\rho, \quad (48)$$

$$V_\rho(x) = \int \phi(x - y) n(y) dy, \quad (49)$$

$$n(y) = \underline{\rho}(y, y). \quad (50)$$

If a pure-state is considered, i.e. if  $\rho = (\cdot, \psi)\psi$  is a projector, then  $\psi$  satisfies the Schrödinger mean-field equation

$$i\hbar\partial_t\psi = \mathcal{H}_{mf}\psi, \quad (51)$$

$$\mathcal{H}_{mf} = \frac{1}{2}|p|^2 + V_\psi, \quad (52)$$

$$V_\psi(x) = \int \phi(x-y)n(y) dy, \quad (53)$$

$$n(y) = |\psi(y)|^2, \quad (54)$$

However, for a more precise mean-field limit, it is important to take into account some more refined statistical properties of the particles. If fermions are considered (which is the case of electrons), the  $N$ -particle wave function is antisymmetric under particle permutations, i.e. :

$$\psi(x_{\sigma(1)}, \dots, x_{\sigma(N)}) = (-1)^{\varepsilon(\sigma)}\psi(x_1, \dots, x_N), \quad (55)$$

where  $\sigma$  is a permutation of  $\{1, \dots, N\}$  and  $\varepsilon(\sigma)$  is the signature of this permutation. Then, the density matrix satisfies

$$\underline{\rho}(x_1, x'_{\sigma(1)}, \dots, x_N, x'_{\sigma(N)}) = (-1)^{\varepsilon(\sigma)}\underline{\rho}(x_1, x'_1, \dots, x_N, x'_N). \quad (56)$$

Clearly, the Hartree mean-field closure (42) does not satisfy this property. The most simple closure which does satisfy this antisymmetry property is the Slater determinant closure:

$$\underline{\rho}^2(x_1, x'_1, x_2, x'_2) = \underline{\rho}^1(x_1, x'_1)\underline{\rho}^1(x_2, x'_2) - \underline{\rho}^1(x_1, x'_2)\underline{\rho}^1(x_2, x'_1). \quad (57)$$

Inserting this closure into (41), we find

$$\underline{Q}^1(\rho^2) \approx (V_\rho(x_1) - V_\rho(x'_1))\underline{\rho}^1(x_1, x'_1) - \underline{Q}_{\text{ex}}(\rho^1), \quad (58)$$

with

$$\underline{Q}_{\text{ex}}(\rho^1) = \int [\phi(x_1 - x_2) - \phi(x'_1 - x_2)]\underline{\rho}^1(x_1, x'_1)\underline{\rho}^1(x_2, x'_1) dx_2. \quad (59)$$

The quantity  $\underline{Q}_{\text{ex}}$  is called the exchange-correlation potential. We can write it shortly:

$$Q_{\text{ex}} = \text{Tr}\{[\phi, (\rho \otimes \rho)_{\text{ex}}]\}_2, \quad (60)$$

with

$$(\rho \otimes \rho)_{\text{ex}} = \underline{\rho}^1(x_1, x'_1)\underline{\rho}^1(x_2, x'_1), \quad (61)$$

and  $\text{Tr}\{\}_2$  is the trace w.r.t the second variable.

Finally, we find the Hartree-Fock mean-field model

$$i\hbar\partial_t\rho = [\mathcal{H}_{mf}, \rho] - Q_{\text{ex}}(\rho), \quad (62)$$

$$\mathcal{H}_{mf} = \frac{1}{2}|p|^2 + V_\rho, \quad (63)$$

$$Q_{\text{ex}} = \text{Tr}\{[\phi, (\rho \otimes \rho)_{\text{ex}}]\}_2, \quad (64)$$

$$V_\rho(x) = \int \phi(x-y)n(y) dy, \quad (65)$$

$$n(y) = \underline{\rho}(y, y). \quad (66)$$

### 2.3 Quantum methods: a brief and incomplete summary

The mean-field limit has first been rigorously proven in the case of a smooth interaction potential  $\phi$  by Spohn [59] and recently in the case of the Coulomb potential by Bardos, Golse, and Mauser [6]. The Hartree-Fock case has been solved by Bardos, Golse, Gottlieb, Mauser in [7, 8].

The existence theory for the Schrödinger mean-field equation has first been developed in the stationary case by Nier [53, 54, 55] and Kaiser and Rehberg [43]. The semiclassical limit  $\hbar \rightarrow 0$  of the Wigner formulation of the density-matrix mean-field equations has been developed by Lions and Paul [47] and by Markowich and Mauser [50].

There is no such thing as a BBGKY hierarchy for Hard-Spheres dynamics in quantum mechanics and so no quantum equivalent of the Boltzmann equation, at least up to our knowledge.

We refer to [44] for a complete monography of up-to-date techniques. Numerical simulations of 'Small' systems (such as atoms, molecules up to a few tens of electrons) have first focused on the eigenvalue problem for finding the minimal energy (lowest eigenvalue of the Hamiltonian) or the excited states (i.e. the lower part of the spectrum of the Hamiltonian). For this purpose, the techniques have primarily concentrated upon the Hartree-Fock (i.e. assuming that the wave-function assumes the form of a Slater determinant) or multi-configuration techniques (i.e. the wave-function is a combination of a finite number of Slater determinants). Usually, for quantum chemistry computations, the Born-Oppenheimer approximation is made. It consists in decoupling the electron and nuclei dynamics based on the small mass ratio of the electrons to the ions and assuming that the ions move classically on quantum mechanically computed electron energy surfaces. To reach convergence of the electron minimization problem for a given configuration of nuclei positions is sometimes very time consuming. This is why Car and Parinello proposed to optimize the nuclei position on the fly, without waiting for the convergence of the electron minimization problem [18].

The dynamical study of small systems is also very important for applications such as chemical reactions dynamics particularly when energy surface crossings are involved or the determination of chemical intermediates is needed. Modern applications of such dynamical problems involve the control of chemical reactions by lasers. Such dynamical studies make use either of

direct computations of the time-dependent Schrödinger equation or that of the time-dependent Hartree-Fock model.

In the case of large systems such as large molecules, crystals, nano-objects or those systems involved in molecular dynamics computations of phase changes, the direct resolution of the Schrödinger equation or time-dependent Hartree-Fock equation is computationally too demanding. Then, Density Functional Theory (DFT) is used. DFT reduces the problem of finding the minimal energy of such a system to the resolution of a one-particle Schrödinger equation in a nonlinear potential which is a functional of the density. This observation is originally due to Hohenberg and Kohn in [39]. Although the method is exact, the functional of the density is not known and various kinds of approximations are needed among which the most popular ones are the Thomas-Fermi and Kohn-Sham models (see e.g. [28]). However, the validity of these approximations is still under scrutiny.

The modeling of open systems such as electrons in a semiconductor, molecules in a solvent, proteins in a biological cell is even more complex. The main question is how to account for the environment of these molecules without having to compute their environment in full detail. Typically, a model for an open system would start with a density matrix formulation of the problem in terms of

$$\underline{\rho}(x_1, x'_1, \dots, x_N, x'_N, y_1, y'_1, \dots, y_P, y'_P)$$

where  $x_1, \dots, x_N$  denote the variables of the system of interest and  $y_1, \dots, y_P$  denote the environment variables. Then, taking the partial trace of the Quantum Liouville equation for  $\rho$  over the  $y$  variables we find an equation for the partial density matrix corresponding to the variables of interest. However two problems with this approach need to be solved. First, in general, the environment variables, their dynamics and their interaction with the system are poorly known. Second, a closure assumption for the environment variables is needed. Such closures are hard to find and usually rely on a thermodynamical equilibrium hypothesis. Still, this approach has been used in a number of cases, such as the electron-phonon in semiconductors where the partial trace over phonon variables is realized, see e.g. the work of Argyres [4]. In this case, this leads to a quite complex 'collision operator' which exhibits nonlocality in space and time and which is very difficult to deal with numerically. Furthermore, the precise domain of validity of the closure is still to be determined. Quantum kinetic models with collisions have been investigated in [5, 30, 31].

A somewhat different route to model such open systems is via hydrodynamic models. Hydrodynamic models are expected to be valid at a meso-scale, i.e. in conditions such that the system is large enough so that a notion of thermodynamic limit is valid while being not too large in order to prevent quantum decoherence to occur. They rely on a scale separation hypothesis, namely that small scale phenomena are clearly separated from large scale ones; small scales are quickly dissipated towards a local thermodynamical equilib-

rium while large scales follow the macroscopic hydrodynamic evolution. We are now going to review the existing attempts in this direction.

## 2.4 Hydrodynamic limits: a review

The difficulty with deriving quantum hydrodynamic models is that there does not exist a kinetic model which would clearly play the role which the Boltzmann equation plays for the derivation of classical hydrodynamic models.

It is known since Madelung that the Schrödinger equation has a formulation in the form of a pressureless gas dynamics equation perturbed by a quantum term. As such, it would describe a single-particle hydrodynamics. It has given rise to the concept of quantum trajectories also known as Bohmian mechanics because it led Bohm to propose a sort of 'deviant' interpretation of quantum mechanics. Now the concept of Bohmian trajectories is routinely used as a numerical integration tool for solving the Schrödinger equation [48], [60].

In the follow-up of this document, we shall propose an extension of this concept to many-particle hydrodynamics by using the entropy minimization principle "à la Levermore" [45].

In the classical case, the single particle hydrodynamics follows from considering the Free Transport equation (where  $f(x, v, t)$  is the distribution function,  $x$  being the position,  $v$ , the velocity and  $t$  the time):

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f - \nabla_x V \cdot \nabla_v f = 0$$

and looking for monophasic solutions of the form

$$f = n(x, t) \delta(v - u(x, t)).$$

Then,  $n$  and  $u$  satisfy exactly the Pressureless gas dynamics:

$$\partial_t n + \nabla_x \cdot nu = 0, \tag{67}$$

$$\partial_t u + u \cdot \nabla_x u = -\nabla_x V. \tag{68}$$

This system has some unpleasant features, such as being non strictly hyperbolic. It has been investigated and used by Brenier and Grenier [12], Bouchut [13], E and coauthors [29], ...

The quantum case follows a similar methodology. We consider a single state  $\psi$  and the associated Schrödinger equation

$$i\hbar \partial_t \psi = -\frac{\hbar^2}{2} \Delta \psi + V(x, t) \psi, \tag{69}$$

and we decompose the wave function into its amplitude  $\sqrt{n}$  and its phase  $S$  as follows:

$$\psi = \sqrt{n} e^{iS/\hbar}. \tag{70}$$

Inserting this Ansatz into (69) and taking real and imaginary parts, we get

$$\partial_t n + \nabla_x \cdot nu = 0, \tag{71}$$

$$\partial_t S + \frac{1}{2} |\nabla S|^2 + V - \frac{\hbar^2}{2} \frac{1}{\sqrt{n}} \Delta \sqrt{n} = 0. \tag{72}$$

Defining  $u = \nabla_x S$  and taking the gradient of the phase equation, we get:

$$\partial_t n + \nabla_x \cdot nu = 0, \tag{73}$$

$$\partial_t u + u \cdot \nabla_x u = -\nabla_x (V + V_B), \tag{74}$$

$$V_B = -\frac{\hbar^2}{2} \frac{1}{\sqrt{n}} \Delta \sqrt{n}. \tag{75}$$

This system appears as the Pressureless Gas Dynamics equations with an additional potential  $V_B$  called the Bohm potential which is an order  $O(\hbar^2)$  term. If this term is neglected, the phase equation leads to the classical Hamilton-Jacobi equation. The Bohm potential involves dispersive term which adds high frequency oscillations and leads to delicate numerics. This model has been mathematically investigated by Markowich and coauthors [37].

Of course, the natural question is whether it is possible to add an energy balance equation which would allow to describe a finite temperature many-particle system. To do so, a straightforward idea is to start for a mixed-state (in the density operator or Wigner distribution formulations), to compute the mass and momentum balance equation for each of the states involved in the mixture and to average over the statistics of the states. But clearly, we are facing a closure problem, since the average in the quantities involved in the mixture are unlikely to be expressed in terms of total mass, momentum and energy only. This closure problem has been solved by various methods in the literature: Gardner [34] has used a classical Fourier law for the heat flux. Gasser, Markowich, Ringhofer [38] have proposed a small temperature asymptotics. Gardner and Ringhofer [35, 36] have developed a Chapman-Enskog expansion for a phenomenological BGK-type collision term. Related approaches can be found in [16, 14, 15, 49].

In these notes, we propose a different approach, based on an entropy minimization principle 'à la Levermore' [45]. This method has been developed in [25].

### 3 Quantum hydrodynamic models derived from the entropy principle

#### 3.1 Quantum setting

In this section, we consider a collisional Quantum Liouville equation

$$i\hbar \partial_t \rho = [\mathcal{H}, \rho] + i\hbar \mathcal{Q}(\rho), \tag{76}$$

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

$$\mathcal{H}\psi = -\frac{\hbar^2}{2}\Delta\psi + V(x, t)\psi, \quad (77)$$

and  $\mathcal{Q}(\rho)$  is an unspecified collision operator which describes the interaction of the particles with themselves and with their environment and accounts for dissipation mechanisms. The only assumption that will be used is that this operator dissipates entropy (see below).

Let  $W[\rho](x, p)$  denote the Wigner transform of  $\rho$ :

$$W[\rho](x, p) = \int \underline{\rho}(x - \frac{1}{2}\xi, x + \frac{1}{2}\xi) e^{i\frac{\xi \cdot p}{\hbar}} d\xi, \quad (78)$$

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

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

Note that we use the momentum  $p$  instead of the velocity  $v$  used in the classical setting. We make  $m = 1$  so that  $v = p$ . We recall that the inverse Wigner transform (or Weyl quantization) is given by the following formula:

$$W^{-1}(w)\psi = \frac{1}{(2\pi)^d} \int w\left(\frac{x+y}{2}, \hbar k\right) \psi(y) e^{ik(x-y)} dk dy, \quad (79)$$

and defines  $W^{-1}(w)$  as an operator acting on the element  $\psi$  of  $L^2$ . The function  $w$  is also called the Weyl symbol of  $\rho$ . Again,  $W$  and  $W^{-1}$  are Isometries between  $\mathcal{L}^2$  (the space of operators such that the product  $\rho\rho^\dagger$  is trace-class, where  $\rho^\dagger$  is the Hermitian conjugate of  $\rho$ ) and  $L^2(\mathbb{R}^{2d})$ :

$$\text{Tr}\{\rho\rho^\dagger\} = \int W[\rho](x, p) \overline{W[\sigma](x, p)} \frac{dx dp}{(2\pi\hbar)^d}. \quad (80)$$

Taking the Wigner transform of (76), we get the following collisional Wigner equation for  $w = W[\rho]$ :

$$\partial_t w + p \cdot \nabla_x w + \Theta^\hbar[V]w = Q(w). \quad (81)$$

with

$$\begin{aligned} \Theta^\hbar[V]w = & -\frac{i}{(2\pi)^d \hbar} \int (V(x + \frac{\hbar}{2}\eta) - V(x - \frac{\hbar}{2}\eta)) \times \\ & \times w(x, q) e^{i\eta \cdot (p-q)} dq d\eta. \end{aligned} \quad (82)$$

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

In the next section, we are going to make use of the entropy dissipation properties of  $Q$  to derive quantum hydrodynamic models.

### 3.2 QHD via entropy minimization

This section is a summary of [25, 26]. A related approach can be found in [46, 52, 61]. We are following Levermore's approach for the classical Boltzmann equation [45]. We take the moments of (76) and close the resulting system by the assumption that  $\mathcal{Q}(\rho)$  relaxes the system to an equilibrium  $\rho_\alpha$  defined as an entropy minimizer constrained to have the same prescribed moments as  $\rho$ . The question is how such an equilibrium is defined.

First, let us define the moments of a quantum system. They are defined like in classical mechanics as the moments of the Wigner distribution function. Let  $\mu_i(p)$ ,  $i = 0, \dots, N$  denote a list of monomial functions of the momentum  $p$  such as e.g the list of hydrodynamic monomials  $(1, p, |p|^2)$ . We denote by  $\mu(p) = (\mu_i(p))_{i=0}^N$  the vector listing all these monomials. We construct a list of moments  $m[w] = (m_i[w])_{i=0}^N$  of moments of  $w$  by setting

$$m_i[w] = \int w(x, p) \mu_i(p) \widetilde{dp}, \quad \widetilde{dp} := \frac{dp}{(2\pi\hbar)^d}. \quad (83)$$

For instance,  $m = (n, q, \mathcal{W})$  (where  $n$  is the local particle density,  $q$  the momentum density and  $\mathcal{W}$  the energy density) in the case of the list of hydrodynamic monomials  $(1, p, |p|^2)$ :

$$\begin{pmatrix} n \\ q \\ 2\mathcal{W} \end{pmatrix} = \int W[\rho] \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} \widetilde{dp}. \quad (84)$$

Note that

$$m_i[\rho](y) = \text{Tr}\{\rho W^{-1}(\mu_i(p)\delta(x-y))\},$$

i.e.  $m_i[\rho](y)$  is the observation of the observable  $\mu_i(p)$  locally at point  $y$ . This definition of the moments is therefore consistent with the quantum definition of an observable.

The moment method now consists in taking the moments of the Wigner equation:

$$\partial_t m[w] + \nabla_x \cdot \int w \mu p \widetilde{dp} + \int \Theta[V]w \mu \widetilde{dp} = \int Q(w) \mu \widetilde{dp}. \quad (85)$$

In general  $\int Q(w) \mu \widetilde{dp} \neq 0$  except for those moments conserved by the collision operator (e.g mass, momentum and energy) in the case of a 'Boltzmann-like' collision operator.

Now, the closure problem reads as follows: find an expression of the integrals by setting  $w$  to be a local thermodynamical equilibrium, i.e. a solution of the entropy minimization problem. Now, we turn to the definition of the quantum entropy.

Recall that the density operator  $\rho$  in its eigenfunction basis  $\phi_s$  reads

$$\rho\psi = \sum_{s \in S} \rho_s(\psi, \phi_s)\phi_s, \quad (86)$$

with

$$0 \leq \rho_s \leq 1, \quad \sum_{s \in S} \rho_s = 1. \quad (87)$$

In this setting, the quantum Boltzmann entropy reads

$$H[\rho] = \sum_{s \in S} \rho_s(\ln \rho_s - 1). \quad (88)$$

It should be noted that the theory can be developed for any entropy, such as the Fermi-Dirac or Bose-Einstein entropy but we restrict ourselves to the Boltzmann entropy for simplicity and refer to [25] for the general case. Here, the entropy is nothing but the information entropy of a system which has discrete states  $\rho_s$ .

Functional calculus tells us how to compute a function of an operator. Let  $h : \mathbb{R} \rightarrow \mathbb{R}$  be an arbitrary function (say continuous to fix the ideas). Then:  $h(\rho)$  is defined by

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

Then, the quantum entropy reads

$$H[\rho] = \text{Tr}\{\rho(\ln \rho - 1)\}. \quad (89)$$

Note that we do not take into account that  $\text{Tr} \rho = 1$  for the time being. We also note that this definition of the entropy is opposite to the usual physical definition. We choose the mathematical convention to prefer convex to concave functions but of course, this unusual convention will not change anything to the results.

Now, the entropy minimization principle reads as follows: Given a set of moments  $m = (m_i(x))_{i=0}^N$ , minimize  $H(\rho)$  subject to the constraint that

$$\int W[\rho](x, p) \mu(p) \widetilde{dp} = m(x) \quad \forall x \in \mathbb{R}^d.$$

As it appears in the formulation of the problem, the entropy is naturally defined in terms of the density operator while the moments are naturally defined in terms of Wigner functions. We now need to reconcile these two representations by invoking the Wigner or inverse Wigner transformations. Because these transformations are non local transformations, the entropy minimization problem must be stated globally (in space) and not locally like in classical mechanics. In other words, we expect that the value of the quantum local thermodynamical equilibrium at one point be dependent on the value of the moments at all points and not specifically at that point like in classical mechanics. This is a signature of the non-local character of quantum mechanics.

We choose to express the moment constraints in terms of the density operator  $\rho$ . For this purpose, we dualize the constraint: Let  $\lambda(x) = (\lambda_i(x))_{i=0}^N$  be an arbitrary (vector) test function. We compute

$$\int w(x, p) \mu(p) \cdot \lambda(x) dx \widetilde{dp} = \int m(x) \cdot \lambda(x) dx, \quad (90)$$

and use (80) to express the left-hand side of this equation in terms of  $\rho$ :

$$\text{Tr}\{\rho W^{-1}[\mu(p) \cdot \lambda(x)]\} = \int m(x) \cdot \lambda(x) dx. \quad (91)$$

Here,  $\mu(p) \cdot \lambda(x)$  for instance denotes  $\sum_{i=0}^N \mu_i(p) \lambda_i(x)$ .

Therefore, the entropy minimization principle has the following expression: given a set of (physically admissible) moments  $m = (m_i(x))_{i=0}^N$ , solve

$$\begin{aligned} \min\{ H[\rho] = \text{Tr}\{\rho(\ln \rho - 1)\} \quad \text{subject to:} \\ \text{Tr}\{\rho W^{-1}[\mu(p) \cdot \lambda(x)]\} = \int m \cdot \lambda dx, \quad \forall \lambda = (\lambda_i(x))_{i=0}^N \}. \end{aligned} \quad (92)$$

To solve this problem, we need to compute the Gâteaux derivative of  $H$ . We have:

$$\frac{\delta H}{\delta \rho} \delta \rho \stackrel{\text{def}}{=} \lim_{t \rightarrow 0} \frac{1}{t} (H[\rho + t \delta \rho] - H[\rho]) = \text{Tr}\{\ln \rho \delta \rho\}. \quad (93)$$

This result has first been given by Nier [53, 54, 55]. An elementary proof can be found in [25].

Now, using this result and the classical Lagrange multiplier technique, we can assert that there exists a set of Lagrange multipliers, which, here, are functions of  $x$ ,  $\alpha(x) = (\alpha_i(x))_{i=0}^N$ , such that:

$$\text{Tr}\{\ln \rho \delta \rho\} = \text{Tr}\{\delta \rho W^{-1}[\mu(p) \cdot \alpha(x)]\}. \quad (94)$$

We deduce that

$$\ln \rho = W^{-1}[\mu(p) \cdot \alpha(x)]. \quad (95)$$

Therefore, the solution of the entropy problem is  $\rho_\alpha$  such that,

$$\rho_\alpha = \exp(W^{-1}[\alpha(x) \cdot \mu(p)]), \quad (96)$$

where  $\alpha = (\alpha_i(x))_{i=0}^N$  is determined such that the moments of  $\rho_\alpha$  are given by  $m$  i.e.  $m[\rho_\alpha] = m$ .

Introducing  $\mathcal{M}_\alpha = W[\rho_\alpha]$  the Wigner transform of  $\rho_\alpha$ , we have

$$\mathcal{M}_\alpha = \mathcal{E}xp(\alpha(x) \cdot \mu(p)), \quad \mathcal{E}xp \cdot = W[\exp(W^{-1}(\cdot))]. \quad (97)$$

The term  $\mathcal{E}xp$  denotes the exponential in the operator sense, i.e. taking a symbol  $w$ , make it an operator using the Weyl quantization, taking the operator exponential and Wigner transforming the resulting operator. It is a

highly nonlinear and non-local operator acting on the function  $w$  and will be referred to as the 'Quantum exponential'. From (97) the analogy between the quantum Local Thermodynamical Equilibrium (LTE) and the classical one given by  $M_\alpha = \exp(\alpha \cdot \mu)$  is clear. The only (but tremendous) difference is the replacement of the classical exponentiation by this new operator exponentiation.

Now, we can close the moment system (85) with the quantum Maxwellian and get

$$\begin{aligned} \partial_t \int \mathcal{E} \exp(\alpha \cdot \mu) \mu dp + \nabla_x \cdot \int \mathcal{E} \exp(\alpha \cdot \mu) \mu p dp \\ + \int \Theta[V] \mathcal{E} \exp(\alpha \cdot \mu) \mu dp = \int Q(\mathcal{E} \exp(\alpha \cdot \mu)) \mu dp. \end{aligned} \quad (98)$$

This gives an evolution system for the vector function  $\alpha(x, t)$  which will be referred to in the sequel as the Quantum Moment Model (QMM). Note that the right-hand side would be identically zero for the hydrodynamic moments (mass, momentum and energy) if the quantum collision operator conserves these quantities.

It is often more informative to use the density operator formulation in (QMM). For this purpose, we transform (QMM) into density operator formalism using (91). We start from the quantum Liouville equation (76), take moments and close with the equilibrium  $\rho = \rho_\alpha$ . This gives

$$\begin{aligned} \partial_t \text{Tr}\{\rho_\alpha W^{-1}(\lambda \cdot \mu)\} = -\frac{i}{\hbar} \text{Tr}\{[\mathcal{H}, \rho_\alpha] W^{-1}(\lambda \cdot \mu)\} \\ + \text{Tr}\{\mathcal{Q}(\rho_\alpha) W^{-1}(\lambda \cdot \mu)\}, \quad \forall \text{ test fct } \lambda(x) = (\lambda_i(x))_{i=0}^N. \end{aligned} \quad (99)$$

Then, using the cyclic property of the trace, we get

$$\begin{aligned} \partial_t \int m[\rho_\alpha] \lambda dx = -\frac{i}{\hbar} \text{Tr}\{\rho_\alpha [W^{-1}(\lambda \cdot \mu), \mathcal{H}]\} + \\ + \text{Tr}\{\mathcal{Q}(\rho_\alpha) W^{-1}(\lambda \cdot \mu)\}, \quad \forall \text{ test fct } \lambda(x) = (\lambda_i(x))_{i=0}^N, \end{aligned} \quad (100)$$

which appears as the weak formulation of (QMM) using density operator formulation.

We now return to the entropy concept. First, we note that the kinetic entropy  $H[\rho]$  in terms of  $w = W[\rho]$  is written

$$H[\rho] = \text{Tr}\{\rho(\ln \rho - 1)\} = \int w(\mathcal{L}n w - 1) dx \widetilde{dp}, \quad (101)$$

where the quantum logarithm is defined analogously as the quantum exponential  $\mathcal{L}n w = W[\ln(W^{-1}(w))]$ .

Now, the fluid entropy is defined as the following function  $S(m)$  of the moments  $m$ :

$$S(m) = H[\rho_\alpha] = \int \mathcal{E}\text{xp}(\alpha \cdot \mu) ((\alpha \cdot \mu) - 1) dx \widetilde{dp}, \quad (102)$$

where  $\alpha$  is such that the moments of  $\mathcal{E}\text{xp}(\alpha \cdot \mu)$  are  $m$  i.e.

$$m[\alpha] := \int \mathcal{E}\text{xp}(\alpha \cdot \mu) \mu dp = m. \quad (103)$$

The fluid entropy is therefore the kinetic entropy evaluated for the equilibrium and considered as a function of the moments. We can show that  $S(m)$  convex. The proof is given in [25] and is a consequence of the convexity of the Boltzmann entropy function  $h(\rho) = \rho(\ln \rho - 1)$ .

Now, with (103), we can write

$$S(m) = \int \alpha \cdot m dx - \Sigma(\alpha), \quad (104)$$

with  $\Sigma(\alpha)$  the Legendre dual of  $S$  (also known as the Massieu-Planck potential):

$$\Sigma(\alpha) = \int \mathcal{E}\text{xp}(\alpha \cdot \mu) dx \widetilde{dp}. \quad (105)$$

$\Sigma(\alpha)$  is also convex and we have the following formulae for the inversion of the mapping  $\alpha \rightarrow m$ :

$$\frac{\delta S}{\delta m} = \alpha, \quad \frac{\delta \Sigma}{\delta \alpha} = m, \quad (106)$$

where the  $\delta$ 's denote Gâteaux derivatives.

We sketch the proof of (106). Using (93), we have

$$\begin{aligned} \delta \Sigma &= \text{Tr}\{ \exp(W^{-1}(\alpha \cdot \mu)) (W^{-1}(\delta \alpha \cdot \mu)) \} \\ &= \int \mathcal{E}\text{xp}(\alpha \cdot \mu) (\delta \alpha \cdot \mu) dx \widetilde{dp} \\ &= \int \delta \alpha \cdot m dx, \end{aligned} \quad (107)$$

which proves the second formula (106).

Now, we have

$$\delta S = \int (\delta \alpha \cdot m + \alpha \cdot \delta m) dx - \delta \Sigma, \quad (108)$$

and with (107) we deduce that

$$\delta S = \int \alpha \cdot \delta m dx, \quad (109)$$

which proves the first formula (106).

If we assume that the collision operator is entropy dissipative, then we can prove that the moment models are compatible with the entropy dissipation, i.e. satisfy:

$$\partial_t S(m(t)) \leq 0, \quad (110)$$

for any solution  $m(t)$  of (QMM).

To prove this result, we use the density matrix formulation of (QMM) (100) or (99) and choose  $\lambda = \alpha$  as a test function:

$$\begin{aligned} \partial_t \int m[\rho_\alpha] \alpha \, dx &= -\frac{i}{\hbar} \text{Tr}\{\rho_\alpha [W^{-1}(\alpha \cdot \mu), \mathcal{H}]\} \\ &\quad + \text{Tr}\{\mathcal{Q}(\rho_\alpha) W^{-1}(\alpha \cdot \mu)\}. \end{aligned} \quad (111)$$

The first term of the left-hand side of (111) is the time derivative of the entropy. Indeed, we have

$$\int m[\rho_\alpha] \alpha \, dx = \text{Tr}\{\rho_\alpha W^{-1}(\alpha \cdot \mu)\} = \text{Tr}\{\rho_\alpha \ln \rho_\alpha\}, \quad (112)$$

and taking the time derivative leads to

$$\partial_t \int m[\rho_\alpha] \alpha \, dx = \partial_t (\text{Tr}\{\rho_\alpha \ln \rho_\alpha\}) = \partial_t (\text{Tr}\{\rho_\alpha (\ln \rho_\alpha - 1)\}) = \partial_t S(m). \quad (113)$$

Here, we have used the fact that  $\text{Tr}\{\rho_\alpha\} = 1$ . Indeed, in this theory, we always normalize the moments by the total mass in order to keep total mass equal to unity (i.e.  $\int n \, dx = 1$ ) and keep the trace of the density matrix equal to unity. The first term at the right-hand side of (111) is transformed using the cyclic invariance of the trace and the fact that two operators such that one is a function of the other one commute (they have the same eigenfunctions):

$$\text{Tr}\{\rho_\alpha [W^{-1}(\alpha \cdot \mu), \mathcal{H}]\} = \text{Tr}\{[\rho_\alpha, \ln \rho_\alpha] \mathcal{H}\} = 0. \quad (114)$$

Finally, we express that  $\mathcal{Q}$  is entropy dissipative:

$$\text{Tr}\{\mathcal{Q}(\rho_\alpha) W^{-1}(\alpha \cdot \mu)\} = \text{Tr}\{\mathcal{Q}(\rho_\alpha) \ln \rho_\alpha\} \leq 0. \quad (115)$$

Collecting (111) to (115) leads to (110) and proves entropy dissipation.

A remarkable special case of (QMM) is the Quantum Hydrodynamic Model (QHD) which is obtained by choosing the set of hydrodynamic monomials  $\mu = \{1, p, |p|^2\}$  to generate an evolution system for the hydrodynamic moments. In this setting, using that the collision operator is supposed to preserve mass, momentum and energy, we find the following balance equations:

$$\partial_t n + \nabla_x \cdot nu = 0, \quad (116)$$

$$\partial_t nu + \nabla_x \Pi = -n \nabla_x V, \quad (117)$$

$$\partial_t \mathcal{W} + \nabla_x \cdot \Phi = -nu \cdot \nabla_x V, \quad (118)$$

with the pressure tensor  $\Pi$  and the energy flux  $\Phi$  given by

$$\Pi = \int \mathcal{E} \exp(\alpha \cdot \mu) p \otimes p \, \widetilde{dp}, \quad (119)$$

$$2\Phi = \int \mathcal{E} \exp(\alpha \cdot \mu) |p|^2 \widetilde{dp}, \quad (120)$$

and

$$\alpha \cdot \mu = A(x) + B(x) \cdot p + C(x)|p|^2, \quad (121)$$

such that

$$\int \mathcal{E}xp(\alpha \cdot \mu) \begin{pmatrix} 1 \\ p \\ |p|^2 \end{pmatrix} \widetilde{dp} = \begin{pmatrix} n \\ q \\ 2\mathcal{W} \end{pmatrix}. \quad (122)$$

$A(x)$  and  $C(x)$  are scalar functions of  $x$  while  $B(x)$  is a vector valued function with values in  $\mathbb{R}^d$ .

By a 'Quantum Maxwellian' we now refer to an equilibrium associated with the prescription of the hydrodynamic moments, i.e.

$$\mathcal{M}_\alpha = \mathcal{E}xp(\alpha \cdot \mu) = W(\exp(W^{-1}(\alpha \cdot \mu))), \quad (123)$$

with  $\alpha \cdot \mu$  given by (121) where  $\alpha = (A, B, C)$  are related with  $(n, nu, \mathcal{W})$  in a non-local way through (122). We note that  $u \neq B/2C$  in general while this is true in the classical case.

The operator  $W^{-1}(\alpha \cdot \mu)$  is a second order differential operator:

$$\begin{aligned} W^{-1}(\alpha \cdot \mu)\psi &= -\hbar^2 \nabla \cdot (C \nabla \psi) \\ &\quad -i\hbar(B \cdot \nabla \psi + (1/2)(\nabla \cdot B)\psi) + (A - (\hbar^2/4)\Delta C)\psi. \end{aligned} \quad (124)$$

To prove this result, we note the following identities:

$$W^{-1}(A) = A, \quad (125)$$

$$W^{-1}(B \cdot p) = -i\hbar(B \cdot \nabla + \frac{1}{2}(\nabla \cdot B)), \quad (126)$$

$$W^{-1}(C|p|^2) = -\hbar^2(C\Delta + \nabla C \cdot \nabla + \frac{1}{4}\Delta C). \quad (127)$$

For instance, to show (126), we use (79) and compute

$$W^{-1}(B \cdot p)\psi = \int B\left(\frac{x+y}{2}\right) \cdot p \psi(y) e^{\frac{ip(x-y)}{\hbar}} \widetilde{dp} dy. \quad (128)$$

Elementary manipulations of Fourier transform lead to

$$\int p e^{\frac{ip(x-y)}{\hbar}} \widetilde{dp} = i\hbar \nabla \delta(y-x). \quad (129)$$

Then

$$\begin{aligned} W^{-1}(B \cdot p)\psi &= i\hbar \int B\left(\frac{x+y}{2}\right) \cdot \nabla \delta(y-x) \psi(y) dy \\ &= -i\hbar \int \nabla_y \cdot (B\left(\frac{x+y}{2}\right)\psi(y)) \delta(y-x) dy \\ &= -i\hbar \left( \frac{1}{2} \nabla \cdot B(x)\psi(x) + B(x) \cdot \nabla \psi(x) \right), \end{aligned} \quad (130)$$

which is the result to be proved. Combining identities (125) to (127), we find (124).

Now, suppose that  $W^{-1}(\alpha \cdot \mu)$  has point spectrum only, i.e. has eigenvalues  $a_s[\alpha]$ , and eigenvectors  $\phi_s[\alpha]$ :

$$W^{-1}(\alpha \cdot \mu) = \sum_s a_s(\cdot, \phi_s) \phi_s, \quad (131)$$

$$\rho_\alpha = \exp(W^{-1}(\alpha \cdot \mu)) = \sum_s e^{a_s}(\cdot, \phi_s) \phi_s. \quad (132)$$

Then, from the fact that  $\text{Tr} \rho_\alpha = 1$ , we deduce that  $\sum_s e^{a_s} = 1$ . It follows that  $a_s < 0$  and  $a_s \xrightarrow{s \rightarrow \infty} -\infty$ . We deduce that  $-W^{-1}(\alpha \cdot \mu)$  must be an elliptic operator which indicates that  $C(x)$  is likely to be non-positive, at least in an important part of the domain. This is to be related to the positivity of the temperature for the classical maxwellian case. Of course, this is not a rigorous proof and the study of operator  $-W^{-1}(\alpha \cdot \mu)$  would require further investigations.

In practice, it is necessary to compute the mapping between the so-called 'entropic variables' ( $A, B, C$ ) and the associated 'conservative variables' ( $n, u, \mathcal{W}$ ). This can be done by a minimization problem thanks to the first formula of (106) and the fact that  $\Sigma$  is convex. This formula can indeed be put in a minimization form

$$\min_\alpha \left\{ \Sigma(\alpha) - \int \alpha \cdot m \, dx \right\}, \quad (133)$$

i.e.

$$\min_\alpha \left\{ \sum_s e^{a_s[\alpha]} - \int \alpha \cdot m \, dx \right\}. \quad (134)$$

This idea is used in practical computations (see e.g. [32, 33]).

### 3.3 Quantum Isothermal Euler model

This part is a summary of [22]. We want to develop a quantum counterpart of the classical isothermal Euler equations. In this setting, the temperature of the medium is fixed and uniform:  $T = \text{Constant}$ . To deal with a constant temperature background, it is necessary to change the entropy into the Free Energy

$$G(\rho) = \text{Tr}\{Th(\rho) + \mathcal{H}\rho\}, \quad (135)$$

$$h(\rho) = \rho(\ln \rho - 1), \quad \mathcal{H} = W^{-1}\left(\frac{|p|^2}{2} + V\right). \quad (136)$$

From now on, we shall omit the  $W^{-1}$ . Any function  $\phi(x, p)$  will be identified to the operator  $W^{-1}(\phi(x, p))$ . Two moments are considered: the density  $n$  and the momentum  $nu$ . The entropy minimization problem reads: To find

$$\min G(\rho) = \min(\text{Tr}\{T\rho(\ln \rho - 1) + \mathcal{H}\rho\}), \quad (137)$$

subject to the moment constraints

$$\text{Tr}\{\rho\phi\} = \int n\phi \, dx, \quad (138)$$

$$\text{Tr}\{\rho W^{-1}(p \cdot \Phi)\} = \int nu \cdot \Phi \, dx, \quad (139)$$

for all (scalar and vector respectively) test functions  $\phi$  and  $\Phi$ .

The solution of the entropy minimization problem must satisfy

$$T \ln \rho + \mathcal{H} = \tilde{A} + \tilde{B} \cdot p. \quad (140)$$

After rearrangement, this is equivalent to

$$\ln \rho = -\frac{H(A, B)}{T}, \quad H(A, B) = \frac{|p - B|^2}{2} + A, \quad (141)$$

with

$$A = V - \tilde{A} - |\tilde{B}|^2/2, \quad B = \tilde{B}. \quad (142)$$

We shall refer to  $H(A, B)$  as a modified Hamiltonian.

The quantum Maxellian in density operator formulation reads

$$\rho_{n, nu} = \exp\left(-\frac{H(A, B)}{T}\right), \quad (143)$$

and in Wigner formulation

$$\mathcal{M}_{n, nu} = \mathcal{E}\exp\left(-\frac{H(A, B)}{T}\right), \quad (144)$$

with  $(A, B)$  related with  $(n, nu)$  by the moment conditions (138), (139). We shall suppose that  $T = 1$  for the sake of simplicity from now on.

Let us consider the moment reconstruction problem and suppose that  $H(A, B)$  has a discrete spectrum with eigenvalues  $\lambda_p(A, B)$  and eigenfunctions  $\psi_p(A, B)$  for  $p = 1, \dots, \infty$ . Then we have

$$n(A, B)(x) = \sum_{p=1}^{\infty} \exp(-\lambda_p(A, B)) |\psi_p(A, B)(x)|^2, \quad (145)$$

$$nu(A, B)(x) = \sum_{p=1}^{\infty} \exp(-\lambda_p(A, B)) \text{Im}(\overline{\hbar\psi_p(A, B)(x)} \nabla \psi_p(A, B)(x)). \quad (146)$$

Indeed, by construction, we have

$$\rho_{n, nu} \cdot = \sum_{p=1}^{\infty} \exp(-\lambda_p(A, B)) (\cdot, \psi_p) \psi_p. \quad (147)$$

Of course, the operator  $\rho$  is diagonal in the basis  $(\psi_p)$ , with diagonal element equal to  $\exp(-\lambda_p(A, B))$ . On the other hand, the multiplication operator by  $\phi$  has matrix element in this basis

$$\phi_{p,p'} = \int \phi \psi_p \overline{\psi_{p'}} dx. \quad (148)$$

Since taking the trace of  $\rho\phi$  amounts to summing up the products of the diagonal elements of the operators  $\rho$  and  $\phi$  respectively (since  $\rho$  is diagonal), we get

$$\text{Tr}\{\rho\phi\} = \sum_{p=1}^{\infty} \exp(-\lambda_p(A, B)) \int \phi |\psi_p|^2 dx. \quad (149)$$

Finally

$$\begin{aligned} n(x_0) &= \text{Tr}\{\rho\delta(x - x_0)\} \\ &= \sum_{p=1}^{\infty} \exp(-\lambda_p(A, B)) |\psi_p(x_0)|^2, \end{aligned} \quad (150)$$

which is (145). A similar computation for  $nu$  would lead to (146).

Now, we can state our first expression of the Quantum Isothermal Euler model. It comes as a special case of the (QHD) model (116)-(118) with the energy equation replaced by the assumption of constant temperature. Therefore, it reads

$$\partial_t n + \nabla \cdot nu = 0, \quad (151)$$

$$\partial_t nu + \nabla \Pi = -n \nabla V, \quad (152)$$

with the pressure tensor  $\Pi$  given by

$$\Pi = \int \mathcal{E} \exp(-H(A, B)) p \otimes p \widetilde{dp}, \quad (153)$$

where the modified Hamiltonian  $H(A, B)$  is given by (141) and  $(A, B)$  is related with  $(n, nu)$  by the moment conditions (145), (146).

Now, our next task is to give a more tractable expression of the pressure tensor  $\Pi$  in terms of  $n, nu, A, B$ . Given a scalar test function  $\phi$ , we can write

$$\begin{aligned} \int (\nabla \Pi) \phi dx &= - \int \Pi \nabla \phi dx \\ &= - \int \mathcal{E} \exp(-H(A, B)) (p \cdot \nabla \phi) p dx \widetilde{dp} \\ &= - \text{Tr}\{\exp(-H(A, B)) W^{-1}((p \cdot \nabla \phi)p)\}. \end{aligned} \quad (154)$$

The idea is to use the commutation with  $H(A, B)$  in order to reduce the degree of the  $p$ -monomial. More specifically, if we succeed in writing

$$(p \cdot \nabla \phi)p = [H(A, B), \mathcal{L}] + \mathcal{N}, \quad (155)$$

where  $\mathcal{N}$  is a polynomial in  $p$  of degree strictly less than 2, then

$$\begin{aligned} \text{Tr}\{\exp(-H(A, B)) (p \cdot \nabla \phi)p\} &= \\ &= \text{Tr}\{\exp(-H(A, B)) [H(A, B), \mathcal{L}]\} \\ &\quad + \text{Tr}\{\exp(-H(A, B)) \mathcal{N}\}. \end{aligned} \quad (156)$$

Using the cyclic property of the trace, we have

$$\begin{aligned} \text{Tr}\{\exp(-H(A, B)) [H(A, B), \mathcal{L}]\} &= \\ &= \text{Tr}\{[\exp(-H(A, B)), H(A, B)]\mathcal{L}\} = 0, \end{aligned} \quad (157)$$

so that

$$\text{Tr}\{\exp(-H(A, B)) (p \cdot \nabla \phi)p\} = \text{Tr}\{\exp(-H(A, B)) \mathcal{N}\}, \quad (158)$$

and the degree in  $p$  of the trace to be evaluated has decreased. It remains to find the convenient operators  $\mathcal{L}$  and  $\mathcal{N}$ . In the present case,  $\mathcal{L}$  will be proportional to  $p\phi$ . Therefore, we turn to the computation of  $[H(A, B), p\phi]$ .

We first note the following commutation relations

$$[\phi, \psi] = 0, \quad (159)$$

$$[p \cdot \Phi, \psi] = -i\hbar(\Phi \cdot \nabla \psi), \quad (160)$$

$$[p \cdot \Phi, p \cdot \Psi] = -i\hbar((\Phi \cdot \nabla)\Psi - (\Psi \cdot \nabla)\Phi) \cdot p, \quad (161)$$

$$[|p|^2/2, \phi] = -i\hbar \nabla \phi \cdot p, \quad (162)$$

$$[|p|^2/2, p\phi] = -i\hbar(\nabla \phi \cdot p)p. \quad (163)$$

We note that commutation decreases the degree in  $p$ .

For instance, we show (160). We first note, after (126) that

$$p \cdot \Phi = -i\hbar(\Phi \cdot \nabla + (\nabla \cdot \Phi)/2). \quad (164)$$

Using that two functions of  $x$  commute, we notice that  $[(\nabla \cdot \Phi), \psi] = 0$  and we are left with

$$\begin{aligned} [\Phi \cdot \nabla, \psi]f &= \Phi \cdot \nabla(\psi f) - \psi \Phi \cdot \nabla f \\ &= (\Phi \cdot \nabla \psi)f, \end{aligned} \quad (165)$$

for an arbitrary test function  $f \in L^2$ .

Now, using formulas (159)-(163), the computation of  $[H(A, B), p\phi]$  is easy and leads to

$$\begin{aligned} [H(A, B), p\phi] &= -i\hbar\{(\nabla \phi \cdot p)p - (B \cdot \nabla \phi)p + \\ &\quad + \phi(\nabla B)p - \phi \nabla(A + |B|^2/2)\}. \end{aligned} \quad (166)$$

Therefore

$$(p \cdot \nabla \phi)p = [H(A, B), \mathcal{L}] + \mathcal{N}, \quad (167)$$

with

$$\mathcal{L} = (i/\hbar)p\phi, \quad (168)$$

$$\mathcal{N} = (B \cdot \nabla \phi)p - \phi(\nabla B)p + \phi\nabla(A + |B|^2/2). \quad (169)$$

Then

$$\begin{aligned} \text{Tr}\{\exp(-H(A, B))(p \cdot \nabla \phi)p\} &= \\ &= \text{Tr}\{\exp(-H(A, B))\mathcal{N}\} \\ &= \text{Tr}\{\exp(-H(A, B))((B \cdot \nabla \phi)p - \phi(\nabla B)p + \phi\nabla(A + |B|^2/2))\}. \end{aligned} \quad (170)$$

Using that  $\exp(-H(A, B))$  satisfies the moment reconstruction problem (138), (139), we obtain

$$\begin{aligned} \text{Tr}\{\exp(-H(A, B))(p \cdot \nabla \phi)p\} &= \\ &= \int ((B \cdot \nabla \phi)nu - \phi(\nabla B)nu + n\phi\nabla(A + |B|^2/2)) dx. \end{aligned} \quad (171)$$

We carry all derivatives outside the test function  $\phi$  by using Green's formula and get:

$$\begin{aligned} \text{Tr}\{\exp(-H(A, B))(p \cdot \nabla \phi)p\} &= \\ &= \int (-\nabla(nu \otimes B) - (\nabla B)nu + n\nabla(A + |B|^2/2))\phi dx. \end{aligned} \quad (172)$$

Finally, according to (154), all this expression equals  $-\int(\nabla \Pi)\phi dx$ . The following final expression of  $\Pi$  is deduced:

$$\nabla \Pi = \nabla(nu \otimes B) + (\nabla B)nu - n\nabla(A + |B|^2/2). \quad (173)$$

We are now ready to provide a second expression of the Quantum Isothermal Euler model:

$$\partial_t n + \nabla \cdot nu = 0, \quad (174)$$

$$\partial_t nu + \nabla(nu \otimes B) + (\nabla B)nu - n\nabla(A + |B|^2/2) = -n\nabla V, \quad (175)$$

where  $(A, B)$  are related with  $(n, nu)$  by the moment reconstruction problem (145), (146).

We now consider the Free energy again. The fluid free energy  $\mathcal{G}(n, nu)$  is defined as the kinetic free energy evaluated on the equilibrium density matrix:

$$\mathcal{G}(n, nu) = G(\rho_{n, nu}). \quad (176)$$

Using (137), we find:

$$\mathcal{G}(n, nu) = \text{Tr}\{\exp(-H(A, B))(-H(A, B) - 1 + \mathcal{H})\}. \quad (177)$$

Now the expression (141) of  $H(A, B)$  leads to

$$\mathcal{G}(n, nu) = \text{Tr}\{\exp(-H(A, B))(B \cdot p - A - |B|^2/2 - 1 + V)\}. \quad (178)$$

Finally, using that  $\exp(-H(A, B))$  satisfies the moment reconstruction problem (138), (139), we obtain

$$\mathcal{G}(n, nu) = \int (nu \cdot B + n(V - A - |B|^2/2 - 1)) dx. \quad (179)$$

By construction, if  $V$  is independent of time, the free energy decays in time

$$\frac{d\mathcal{G}}{dt} \leq 0, \quad (180)$$

with equality for smooth solutions. The proof follows the same steps as for the general (QMM) model. If  $V$  solves Poisson equation  $-\Delta V = n$  then, again the entropy inequality (180) holds with a modification of the entropy (179), multiplying the term  $nV$  by a factor 1/2 (a usual procedure when computing self-energies). This shows that the Quantum Isothermal Euler system is compatible with free-energy dissipation.

We now turn to a property of the Quantum Isothermal Euler which is a form of gauge invariance. Let  $S(x)$  be a smooth function. Then

$$\exp\left(\frac{iS}{\hbar}\right) H(A, B) \exp\left(-\frac{iS}{\hbar}\right) = H(A, B + \nabla S). \quad (181)$$

To prove this identity, we write that

$$\begin{aligned} \exp(iS/\hbar)H(A, B) \exp(-iS/\hbar) - H(A, B) &= \\ &= \exp(iS/\hbar)[H(A, B), \exp(-iS/\hbar)], \end{aligned}$$

and we use the commutation relations (159)-(163).

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

$$\exp\left(\frac{iS}{\hbar}\right) \exp(-H(A, B)) \exp\left(-\frac{iS}{\hbar}\right) = \exp(-H(A, B + \nabla S)). \quad (182)$$

Thus, the equilibrium density operators are conjugate. Therefore, the eigenvalues of  $\exp(-H(A, B))$  and  $\exp(-H(A, B + \nabla S))$  are also the same.

Going back to the fluid Free energy (176), formula (179) implies that

$$\frac{\delta\mathcal{G}}{\delta n} = V - A - |B|^2/2 = \tilde{A}, \quad (183)$$

$$\frac{\delta\mathcal{G}}{\delta(nu)} = B. \quad (184)$$

These formulas are direct consequences of (106). The Legendre dual of the entropy is given by

$$\tilde{\Sigma}(\tilde{A}, B) = \int n dx = \text{Tr}\{\exp(-H(A, B))\} := \Sigma(A, B). \quad (185)$$

The inversion formula (106) and the chain rule leads to

$$n(A, B) = \frac{\delta \tilde{\Sigma}}{\delta \tilde{A}} = -\frac{\delta \Sigma}{\delta A}, \quad (186)$$

$$(nu)(A, B) = \frac{\delta \tilde{\Sigma}}{\delta B} = \frac{\delta \Sigma}{\delta B} - B \frac{\delta \Sigma}{\delta A}. \quad (187)$$

It results:

$$\frac{\delta \Sigma}{\delta A} = -n(A, B), \quad (188)$$

$$\frac{\delta \Sigma}{\delta B} = (nu)(A, B) - n(A, B) B. \quad (189)$$

Now, by the gauge invariance, the eigenvalues of  $\exp(-H(A, B))$  and  $\exp(-H(A, B + \nabla S))$  are the same:

$$\begin{aligned} \Sigma(A, B) &= \text{Tr}\{\exp(-H(A, B))\} = \\ &= \text{Tr}\{\exp(-H(A, B + \nabla S))\} = \Sigma(A, B + \nabla S). \end{aligned} \quad (190)$$

This implies

$$\begin{aligned} \frac{\delta \Sigma}{\delta A}(A, B + \nabla S) &= \frac{\delta \Sigma}{\delta A}(A, B), \\ \frac{\delta \Sigma}{\delta B}(A, B + \nabla S) &= \frac{\delta \Sigma}{\delta B}(A, B). \end{aligned}$$

With (188), (189), this leads to

$$n(A, B + \nabla S) = n(A, B), \quad (191)$$

$$(nu)(A, B + \nabla S) = nu(A, B) + n(A, B)\nabla S, \quad (192)$$

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

Another consequence is that for all test functions  $S(x)$ , we have

$$\begin{aligned} \lim_{t \downarrow 0} t^{-1}(\Sigma(A, B + t\nabla S) - \Sigma(A, B)) &= 0 = \\ &= \int \frac{\delta \Sigma}{\delta B} \cdot \nabla S dx = \int (nu - nB) \cdot \nabla S dx, \end{aligned} \quad (193)$$

meaning that

$$\nabla \cdot (n(u - B)) = 0. \quad (194)$$

This expresses the very strong result that  $u$  and  $B$  are not equal but differ by a vector field which is a curl divided by the density.

Now, we are ready to propose various equivalent formulations of the momentum equation originally given by (175). First using that  $\nabla|B|^2/2 = (\nabla B)B$ , we can transform (175) into

$$\partial_t nu + \nabla(nu \otimes B) + n(\nabla B)(u - B) + n\nabla(V - A) = 0. \quad (195)$$

Now, using the constraint (194), we can transform (195) into

$$\begin{aligned} \partial_t nu + \nabla(nu \otimes u) + n(\nabla \times u) \times (B - u) + \\ + n\nabla(V - A - |B - u|^2/2) = 0. \end{aligned} \quad (196)$$

Finally, the continuity equation allows us to transform (195) into

$$\partial_t u + (\nabla \times u) \times B + \nabla(u \cdot B - |B|^2/2 + V - A) = 0. \quad (197)$$

The case of irrotational flows deserves a special mention. We define the vorticity by  $\omega = \nabla \times u$ . By taking the curl of Form (197),  $\omega$  satisfies

$$\partial_t \omega + \nabla \times (\omega \times B) = 0. \quad (198)$$

If  $\omega|_{t=0} = 0$ , then  $\omega \equiv 0$  for all times. Therefore, if a flow is irrotational at time  $t = 0$ , it stays irrotational for all time.

For an irrotational flow, there exists a scalar function  $S(x, t)$  such that  $u = \nabla S$ . Then, it can be proven that

$$u = B = \nabla S. \quad (199)$$

To show this property, we first note that  $nu(A, 0) = 0$ . Indeed,

$$nu(A, 0) = \int \mathcal{E}xp(-H(A, 0))p \widetilde{d}p. \quad (200)$$

But  $H(A, 0) = |p|^2/2 + A$  is even with respect to  $p$ . It follows that  $\mathcal{E}xp(-H(A, 0))$  is also even with respect to  $p$ . This is not obvious (since  $\mathcal{E}xp$  is not the exponential in the usual sense). To prove it, we can write the series expansion of the operator exponential, prove the evenness property for powers of the operator (using Wigner transform for instance) and then extend it by means of the series expansion, to the exponential. It follows that  $nu(A, 0) = 0$  by symmetry.

Now, using the Gauge transformation, we have

$$\begin{aligned} nu(A, \nabla S) &= nu(A, 0) + n(A, 0)\nabla S \\ &= 0 + n(A, \nabla S)\nabla S, \end{aligned}$$

which shows that the solution  $(A, B)$  of the moment problem is given by  $A$  solving  $n(A, 0) = n$  and  $B = \nabla S = u$ . Of course, this argument relies on the

assumption that the pair  $(A, B)$  is unique (given  $(n, nu)$ ), which has not been rigorously proven yet. Therefore, at this point this argument is only formal.

Nevertheless, applying (199) considerably simplifies the formulation of the Quantum Isothermal Euler model in the case of irrotational flows. This system reads (take  $B = u$  in (196)):

$$\partial_t n + \nabla \cdot nu = 0, \quad (201)$$

$$\partial_t nu + \nabla(nu \otimes u) + n\nabla(V - A) = 0, \quad (202)$$

$$\nabla \times u = 0, \quad (203)$$

where  $A$  is related with  $n$  by (145). In this case, only one quantity  $A$  is to be determined from the spectral problem. An important sub-case of irrotational flows is of course one-dimensional flows.

Now, we turn to the semiclassical asymptotics of the Quantum Isentropic Euler model. When  $\hbar \rightarrow 0$ , we recover the classical isothermal Euler equations. If we retain terms of order  $\hbar^2$ , we obtain:

$$\partial_t n + \nabla \cdot (nu) = 0, \quad (204)$$

$$\begin{aligned} \partial_t(nu) + \nabla(nu \otimes u) + \nabla n + n\nabla V - \frac{\hbar^2}{6}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) + \\ + \frac{\hbar^2}{12}\omega \times (\nabla \times (n\omega)) + \frac{\hbar^2}{24}n\nabla(|\omega|^2) = 0, \end{aligned} \quad (205)$$

$$\omega = \nabla \times u. \quad (206)$$

This expansion has been given by Jüngel and Matthes in [40]. The computations leading to these formula are quite involved and we refer the reader to [22].

In the case of irrotational flows  $\omega = 0$ , the semiclassical asymptotics leads to

$$\partial_t n + \nabla \cdot nu = 0, \quad (207)$$

$$\partial_t nu + \nabla(nu \otimes u) + \nabla n + n\nabla V - \frac{\hbar^2}{6}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = 0 \quad (208)$$

This model can be found in the literature under the name of 'Quantum Hydrodynamic Model' [34]. It is a classical isothermal Euler model with the addition of the Bohm potential in the momentum equation. However, in the literature, it is derived on the basis of phenomenological considerations, and is used in the irrotational as well as the non-irrotational cases. Here, this 'Quantum Hydrodynamic Model' is derived on the basis of first principles and it appears to be restricted to irrotational flows, the completely general form valid for non-irrotational flows being (204)-(206).

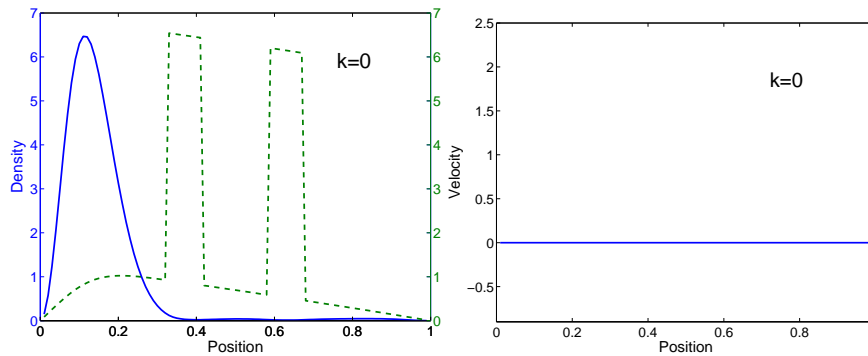
We now report on preliminary numerical results using this model. Our test problem is a one-dimensional model where the hydrodynamic quantities are coupled with Poisson's equation. A relaxation term has been also added to

the momentum relaxation term. We consider a double barrier structure with boundary conditions of Dirichlet type for the wave-function (and consequently for the density) and a zero flux boundary condition for the momentum. We observe the dynamics of electrons which are initially close to the left boundary and which move to eventually fill in the whole domain.

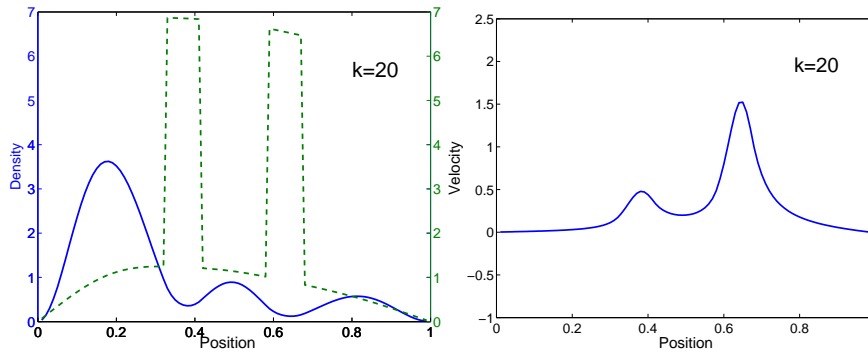
The values of the parameters are given in table 1. The initial density and velocity are depicted in Figure 1. Figures 2, 3 and 4 show the evolution of the electron density on the left, and the velocity on the right after 20, 100 and 200 time steps. We can see electrons going through the barriers by tunneling effect. At time step 200 the system seems to achieve an equilibrium. This is confirmed by Figure 5 which shows that the free energy does not evolve any more. On this last graph, we can see that the free energy is a decreasing function of time, as expected.

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

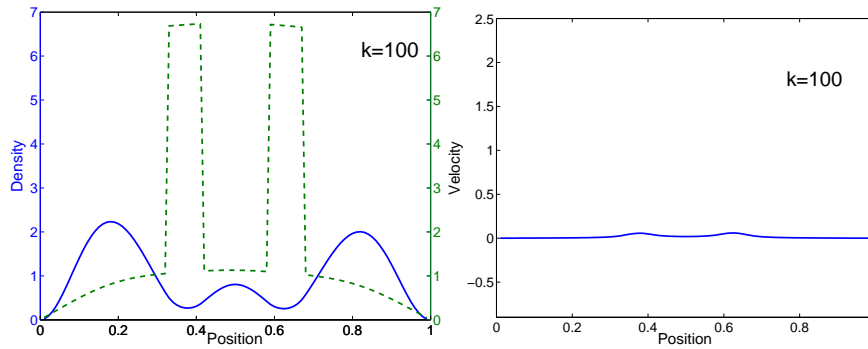
**Table 1.** Values of the parameters for the numerical simulation ( $\Delta x$  is the space step,  $\Delta t$ , the time step,  $\hbar^2/2T$  the scaled Planck constant,  $\alpha$  the scaled Debye length,  $\tau$  the scaled momentum relaxation time, see [22] for the meaning of these parameters)



**Fig. 1.** Numerical solution of the quantum Euler model with relaxation: Initial data. Left: initial density (solid line) and total electrical potential (dashed line) as functions of the position  $x$ . Right: Initial velocity as a function of the position  $x$ .



**Fig. 2.** Numerical solution of the quantum Euler model with relaxation after 20 iterations. Left: density (solid line) and total electrical potential (dashed line) as functions of the position  $x$ . Right: Velocity as a function of the position  $x$ .



**Fig. 3.** Numerical solution of the quantum Euler model with relaxation after 100 iterations. Left: density (solid line) and total electrical potential (dashed line) as functions of the position  $x$ . Right: Velocity as a function of the position  $x$ .

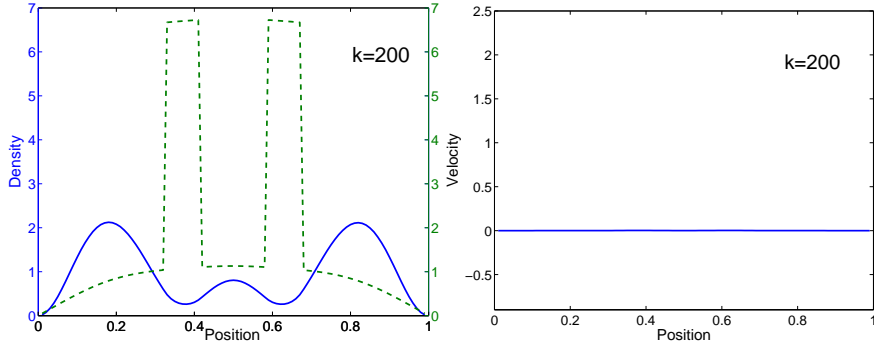
## 4 Quantum diffusion models

### 4.1 Quantum energy-Transport model

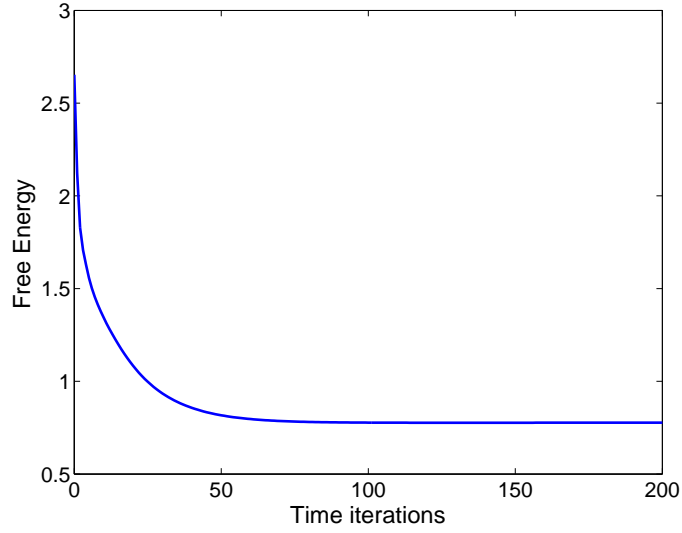
In this section, we report on the work [23, 24].

We notice that the derivation of the Quantum Moment Models, or Quantum Hydrodynamic models did not require any knowledge of the exact form of the collision operator. The only properties which were used were the entropy dissipation and the conservation properties of mass, momentum and energy.

For deriving a diffusion model from a kinetic equation however, the exact form of the collision operator matters and the coefficients of the diffusion model itself depend on this collision operator.



**Fig. 4.** Numerical solution of the quantum Euler model with relaxation after 200 iterations. Left: density (solid line) and total electrical potential (dashed line) as functions of the position  $x$ . Right: Velocity as a function of the position  $x$ .



**Fig. 5.** Evolution of the free energy as a function of the time iteration  $k$ .

Therefore, in order to derive Quantum Diffusion model, we need to specify the collisions operator  $\mathcal{Q}$  in Quantum Liouville equation

$$i\hbar\partial_t\rho = [\mathcal{H}, \rho] + i\hbar\mathcal{Q}(\rho), \quad (209)$$

or in the Wigner equation

$$\partial_t w + p \cdot \nabla_x w + \Theta^{\hbar}[V]w = Q(w). \quad (210)$$

In the absence of a precise definition of the physical collision mechanism, the most simple choice is a relaxation operator also called BGK operator.

The collision operator expresses the relaxation of the collision operator to the Local Thermodynamical Equilibrium, in our case, the quantum Maxwellian. We want to investigate a case where this collision operator is written

$$Q(w)(p) = -\nu(w - \mathcal{E}\text{xp}(A + C|p|^2/2)), \quad (211)$$

where we recall that  $\mathcal{E}\text{xp } w = W(\exp(W^{-1}w))$ . The functions  $A(x)$  and  $C(x)$  are such that the operator  $Q$  locally conserves mass and energy. More precisely, let us write

$$\mathcal{M}_{n,\mathcal{W}} = \mathcal{E}\text{xp}(A + C|p|^2/2), \quad (212)$$

the Quantum Maxwellian whose local mass at point  $x$  is  $n(x)$  and local energy is  $\mathcal{W}(x)$ . Then,  $(A, C)$  is such that

$$\int \mathcal{E}\text{xp}(A + C|p|^2/2) \begin{pmatrix} 1 \\ |p|^2/2 \end{pmatrix} \widetilde{dp} = \begin{pmatrix} n \\ \mathcal{W} \end{pmatrix}. \quad (213)$$

In density operator form, the Quantum Maxwellian is written

$$\rho_{n,\mathcal{W}} = W^{-1}(\mathcal{M}_{n,\mathcal{W}}) = \exp(W^{-1}(A + C|p|^2/2)), \quad (214)$$

with, for all test functions  $\phi$ :

$$\text{Tr}\{\rho_{n,\mathcal{W}} \phi\} = \int n\phi \, dx, \quad \text{Tr}\{\rho_{n,\mathcal{W}} \phi|p|^2/2\} = \int \mathcal{W}\phi \, dx. \quad (215)$$

Again, we recall that the Quantum Maxwellian  $\rho_{n,\mathcal{W}} = \exp(W^{-1}(A + C|p|^2/2))$  is a solution of the entropy minimization principle: to find

$$\begin{aligned} \min \{H[\rho] = \text{Tr}\{\rho(\ln \rho - 1)\}, \quad \text{subject to:} \\ \text{Tr}\{\rho_{n,\mathcal{W}} \phi\} = \int n\phi \, dx, \quad \text{Tr}\{\rho_{n,\mathcal{W}} \phi|p|^2/2\} = \int \mathcal{W}\phi \, dx \}. \end{aligned} \quad (216)$$

In Wigner form, the quantum entropy  $H[\rho]$  has the expression:

$$H[\rho] = \text{Tr}\{\rho(\ln \rho - 1)\} = \int w(\mathcal{L}\text{n } w - 1) \, dx \, \widetilde{dp}, \quad (217)$$

where the quantum logarithm is defined according to  $\mathcal{L}\text{n } w = W[\ln(W^{-1}(w))]$ .

For a given Wigner distribution  $w$ , let us denote by  $\mathcal{M}_w := \mathcal{M}_{n,\mathcal{W}}$  the Quantum Maxwellian which possesses the same density  $n$  and energy  $\mathcal{W}$  as  $w$ :

$$\int \mathcal{M}_w \begin{pmatrix} 1 \\ |p|^2/2 \end{pmatrix} dp = \int w \begin{pmatrix} 1 \\ |p|^2/2 \end{pmatrix} dp. \quad (218)$$

Then, the Quantum BGK operator is written

$$Q(w) = -\nu(w - \mathcal{M}_w). \quad (219)$$

In density operator form, we shall denote the quantum Maxwellian which has the same mass and energy as  $\rho$  by  $\mathcal{M}_\rho$ . Then the Quantum BGK operator is written

$$\mathcal{Q}(\rho) = -\nu(\rho - \mathcal{M}_\rho). \quad (220)$$

The physical situation modeled by  $Q(w)$  is typically when the energy exchanges among the particles themselves are more efficient than with the surrounding and that a different temperature than that of the background is possible. In short channel transistors, the electron typical energy exceeds the phonon energy by almost two orders of magnitude. Then, the phonon collisions can be viewed as quasi-elastic and most of the energy exchanges are with the other electrons via Coulomb interaction. In plasmas, a similar situation arises between electrons and ions because of the very small electron to ion mass ratio.

Again, we observe that we need the two sets of variables: the conservative variables  $(n, \mathcal{W})$  and the entropic variables  $(A, C)$ . The passage between  $(n, \mathcal{W})$  and  $(A, C)$  is a functional change of variable which is done through the entropy and its Legendre dual as seen in the previous sections.

Let us now summarize the properties of  $Q$ :

(i) Mass and energy conservation

$$\int Q(w) \left( \frac{1}{|p|^2} \right) dp = 0, \quad (221)$$

(ii) Null set of  $Q$  (equilibria) :

$$Q(w) = 0 \iff \exists (A, C) \text{ such that } w = \mathcal{E}xp(A + C|p|^2/2), \quad (222)$$

(iii) Entropy decay:

$$\int Q(w) \mathcal{L}n w dx \widetilde{dp} = \text{Tr}\{\mathcal{Q}(\rho) \ln \rho\} \leq 0. \quad (223)$$

Properties (i) and (ii) are obvious from definition (219) and the conservation relations (213). The only delicate point is entropy decay (iii). In the classical case, the proof uses that the logarithm is an increasing function. This is no more true here in the case of the quantum logarithm. Indeed, because the dependence between  $w$  and  $\mathcal{L}n(w)$  is functional, the statement that  $\mathcal{L}n(w)$  is increasing w.r.t  $w$  is meaningless. So another proof must be developed. It uses convexity argument. Indeed, because of the convexity of the entropy functional  $H$ , the function  $A$ :

$$\lambda \in [0, 1] \rightarrow A(\lambda) = H((1 - \lambda)\mathcal{M}_\rho + \lambda\rho), \quad (224)$$

is convex. Therefore,

$$\frac{dA}{d\lambda}(1) \geq A(1) - A(0), \quad (225)$$

follows. From (93), we deduce

$$\frac{d\Lambda}{d\lambda}(\lambda) = \text{Tr}\{\ln((1-\lambda)\mathcal{M}_\rho + \lambda\rho)(\rho - \mathcal{M}_\rho)\}, \quad (226)$$

and in particular that

$$\frac{d\Lambda}{d\lambda}(1) = \text{Tr}\{\ln\rho(\rho - \mathcal{M}_\rho)\} \geq H(\rho) - H(\mathcal{M}_\rho). \quad (227)$$

But, the fact that  $\mathcal{M}_\rho$  solves the entropy minimization principle provides us with

$$H(\rho) - H(\mathcal{M}_\rho) \geq 0, \quad (228)$$

out of which we obtain that

$$\text{Tr}\{\mathcal{Q}(\rho) \ln\rho\} = -\nu \text{Tr}\{\ln\rho(\rho - \mathcal{M}_\rho)\} \leq 0, \quad (229)$$

which is the result to be proven.

Now, we consider a diffusion scaling of the collisional Wigner equation:

$$\eta^2 \frac{\partial w^\eta}{\partial t} + \eta(v \cdot \nabla_x w^\eta - \Theta(w^\eta)) = Q(w^\eta), \quad (230)$$

This scaling is obtained through the change  $t \rightarrow t/\eta$  and  $Q \rightarrow Q/\eta$  which means that the collision operator is large and that we are looking at long time scales.

The limit  $\eta \rightarrow 0$  of (230) is the so-called Quantum Energy-Transport model. Indeed, as  $\eta \rightarrow 0$ ,  $w^\eta \rightarrow \mathcal{E}\exp(A + C|p|^2/2)$  where  $(A, C)$  satisfy the Energy-Transport model which consists of the mass and energy conservation equations

$$\frac{\partial n}{\partial t} + \nabla_x \cdot j_n = 0, \quad (231)$$

$$\frac{\partial \mathcal{W}}{\partial t} + \nabla_x \cdot j_{\mathcal{W}} + \nabla_x V \cdot j_n = 0, \quad (232)$$

where  $(n, \mathcal{W})$  is related with  $(A, C)$  through

$$\int \mathcal{E}\exp(A + C|p|^2/2) \begin{pmatrix} 1 \\ |p|^2/2 \end{pmatrix} \widetilde{dp} = \begin{pmatrix} n \\ \mathcal{W} \end{pmatrix}, \quad (233)$$

and the fluxes  $(j_n, j_{\mathcal{W}})$  are given by

$$j_n = -\nu^{-1}[\nabla \Pi + n \nabla V], \quad (234)$$

$$j_{\mathcal{W}} = -\nu^{-1}[\nabla \mathcal{Q} + (\mathcal{W} \text{Id} + \Pi) \nabla V - \frac{\hbar^2}{8} n \nabla(\Delta V)], \quad (235)$$

with the tensors  $\Pi(A, C)$  and  $\mathcal{Q}(A, C)$  given by

$$H(A, C) = \int \mathcal{E}xp(A + C|p|^2/2) p \otimes p \widetilde{dp}, \quad (236)$$

$$Q(A, C) = \int \mathcal{E}xp(A + C|p|^2/2) p \otimes p |p|^2/2 \widetilde{dp}. \quad (237)$$

Like in the classical case (see e.g. [20, 9, 10]), the system consists of balance equations for the conservative variables  $(n, \mathcal{W})$ , the fluxes of which are expressed in terms of the gradients of the entropic variables  $(A, C)$ . The passage  $(n, \mathcal{W})$  to  $(A, C)$  can be done through the use of the entropy functional or its Legendre dual. However, by contrast with the classical case, there is no clear symmetric positive-definite matrix structure relation between the fluxes and the gradients of the entropic variables.

Let us now consider entropy decay. The fluid entropy is given by the kinetic entropy evaluated for the equilibrium:  $S(n, \mathcal{W}) = H(\mathcal{M}_{n, \mathcal{W}})$  and has the following expressions:

$$\begin{aligned} S(n, \mathcal{W}) &= \int \mathcal{M}_{n, \mathcal{W}} (\mathcal{L}n \mathcal{M}_{n, \mathcal{W}} - 1) dx \widetilde{dp} \\ &= \int \mathcal{E}xp(A + C|p|^2/2) (A + C|p|^2/2 - 1) dx \widetilde{dp} \\ &= \int (n(A - 1) + C\mathcal{W}) dx. \end{aligned} \quad (238)$$

The Quantum Energy-Transport model decreases the entropy:

$$\frac{d}{dt} S(n, \mathcal{W}) \leq 0. \quad (239)$$

The proof follows exactly the same arguments as for the hydrodynamic model and is omitted.

We now sketch how we prove (formally) that the collisional Wigner equation converges in the diffusive limit  $\eta \rightarrow 0$  towards the Quantum Energy-Transport model. The (formal) proof follows three steps.

- (i) Step 1: show that  $w^\eta$  converges to a Quantum Maxwellian  $\mathcal{E}xp(A + C|p|^2/2)$  where  $(A, C) = (A, C)(x, t)$ . Use a Chapman-Enskog expansion to define the first order corrector  $w_1$
- (ii) Step 2: Write mass and energy conservation equations
- (iii) Step 3: Compute the fluxes taking the appropriate moment of  $w_1$

We now give more detail about these three points.

- (i) Step 1: Convergence to equilibrium. Let us suppose that  $w^\eta \rightarrow w$  smoothly. Then, using the Wigner-BGK equation (230) we get  $Q(w^\eta) = O(\eta)$  and consequently  $Q(w) = 0$ , which, thanks to (222), gives  $w = \mathcal{E}xp(A + C|p|^2/2)$ . Now, we can write a Chapman-Enskog like expansion

$$w^\eta = \mathcal{M}_{w^\eta} + \eta w_1^\eta. \quad (240)$$

This expression defines  $w_1^\eta$  and the equal sign is exact. Then:

$$\frac{1}{\eta}Q(w^\eta) = -\nu w_1^\eta = \mathcal{T}w^\eta + \eta\partial_t w^\eta, \quad (241)$$

with

$$\mathcal{T}w = v \cdot \nabla_x w - \Theta^h[V]w, \quad (242)$$

is the transport operator. Therefore, as  $\eta \rightarrow 0$ :

$$w_1^\eta \rightarrow w_1 = -\nu^{-1}\mathcal{T}w, \quad (243)$$

showing that  $w_1^\eta$  has a finite limit.

(ii) Step 2: Mass and energy balance equations. We take the moments of the Wigner-BGK equation against 1 and  $|p|^2/2$ , use that  $Q$  preserves mass and energy and get

$$\frac{\partial n^\eta}{\partial t} + \nabla_x \cdot j_n^\eta = 0, \quad (244)$$

$$\frac{\partial \mathcal{W}^\eta}{\partial t} + \nabla_x \cdot j_{\mathcal{W}}^\eta + \nabla_x V \cdot j_n^\eta = 0, \quad (245)$$

with

$$j_n^\eta = \eta^{-1} \int w^\eta p \widetilde{dp} = \int w_1^\eta p \widetilde{dp}, \quad (246)$$

$$j_{\mathcal{W}}^\eta = \eta^{-1} \int w^\eta p |p|^2/2 \widetilde{dp} = \int w_1^\eta p |p|^2/2 \widetilde{dp}. \quad (247)$$

As  $\eta \rightarrow 0$

$$j_n^\eta \rightarrow j_n = \int w_1 p \widetilde{dp}, \quad (248)$$

$$j_{\mathcal{W}}^\eta \rightarrow j_{\mathcal{W}} = \int w_1 p |p|^2/2 \widetilde{dp}. \quad (249)$$

Therefore, the mass and energy balance equations (244) and (245) are valid in the limit  $\eta \rightarrow 0$  and lead to (231) and (232).

(iii) Step 3: Equations for the fluxes. We start with the equation for  $j_n$ . From (243) and (240), we compute:

$$w_1 = -\nu^{-1}[\nabla_x \cdot (p \mathcal{E} \exp(A + C|p|^2/2)) - \Theta^h[V] \mathcal{E} \exp(A + C|p|^2/2)]. \quad (250)$$

Then

$$\begin{aligned} j_n &= \int w_1 p \widetilde{dp} \\ &= -\nu^{-1}[\nabla \cdot (\int \mathcal{E} \exp(A + C|p|^2/2) p \otimes p \widetilde{dp}) \\ &\quad - \int \Theta^h[V](\mathcal{E} \exp(A + C|p|^2/2)) p \widetilde{dp}]. \end{aligned} \quad (251)$$

For the moments of the field operator  $\Theta^{\hbar}[V]$ , easy computations show that

$$\int \Theta^{\hbar}[V]w \begin{pmatrix} 1 \\ p \\ |p|^2/2 \end{pmatrix} \widetilde{dp} = \begin{pmatrix} 0 \\ -n\nabla V \\ -nu \cdot \nabla V \end{pmatrix}, \quad (252)$$

and

$$\int \Theta^{\hbar}[V]w|p|^2/2p \widetilde{dp} = -(\mathcal{W}\text{Id} + \Pi)\nabla V + \frac{\hbar^2}{8}n \nabla(\Delta V). \quad (253)$$

Using these formulas, we finally find

$$j_n = -\nu^{-1}[\nabla\Pi + n\nabla V], \quad (254)$$

which is the formula to be proved.

Now, we turn to the computation of  $j_{\mathcal{W}}$ . Similar computation give:

$$\begin{aligned} j_{\mathcal{W}} &= \int w_1 p |p|^2/2 dp \\ &= -\nu^{-1}[\nabla(\int \mathcal{E}\text{xp}(A + C|p|^2/2)p \otimes p |p|^2/2 \widetilde{dp}) \\ &\quad - \int \Theta^{\hbar}[V](\mathcal{E}\text{xp}(A + C|p|^2/2)) p |p|^2/2 \widetilde{dp}]. \end{aligned} \quad (255)$$

Using (252) and (253)

$$j_{\mathcal{W}} = -\nu^{-1}[\nabla\mathbb{Q} + (\mathcal{W}\text{Id} + \Pi)\nabla V - \frac{\hbar^2}{8}n \nabla(\Delta V)], \quad (256)$$

which is again the formula to be proven and closes the formal proof that the collisional Wigner equation converges in the diffusive limit towards the Quantum Energy-Transport model.

We now look at the  $\hbar$  expansion of the model up to order  $O(\hbar^2)$ . Again, the computations that lead to these formulae can be found in [23]. The expansion of  $\Pi$  is

$$\begin{aligned} \Pi_{rs} &= \delta_{rs} n T \\ &+ \frac{\hbar^2}{12d} n \delta_{rs} (\Delta_x \ln n + 2\Delta_x \ln T + 2\nabla_x \ln n \cdot \nabla_x \ln T - \frac{d+2}{2} |\nabla_x \ln T|^2) \\ &+ \frac{\hbar^2}{12} n (-\partial_{rs}^2 \ln n - 2\partial_{rs}^2 \ln T - \partial_r \ln n \partial_s \ln T \\ &\quad - \partial_r \ln T \partial_s \ln n + \frac{d+2}{2} \partial_r \ln T \partial_s \ln T), \end{aligned} \quad (257)$$

with  $T = 2W/(dn)$ . The expansion of  $\mathbb{Q}$  gives:

$$\begin{aligned}
\mathbb{Q}_{rs} &= \frac{d+2}{2} \delta_{rs} n T^2 \\
&+ \frac{\hbar^2}{24d} n T \delta_{rs} (\Delta_x \ln n + (d+8) \Delta_x \ln T \\
&\quad + 2(d+4) \nabla_x \ln n \cdot \nabla_x \ln T + \frac{d^2-4d-8}{2} |\nabla_x \ln T|^2) \\
&+ \frac{\hbar^2}{24} (d+4) n T (-\partial_{rs}^2 \ln n - 3\partial_{rs}^2 \ln T \\
&\quad - \partial_r \ln n \partial_s \ln T - \partial_r \ln T \partial_s \ln n + \frac{d}{2} \partial_r \ln T \partial_s \ln T).
\end{aligned} \tag{258}$$

These expressions are quite complicated but if a small temperature variation assumption is made:

$$|\nabla \ln T|/|\nabla \ln n| \ll 1, \tag{259}$$

the model simplifies and gives the following formulae for the fluxes

$$\begin{aligned}
J^n &= -\nabla \left( n T + \frac{\hbar^2}{12d} n \Delta \ln n \right) - n \nabla (V + V_B[n]), \\
J^w &= -\nabla \left( \frac{d+2}{2} n T^2 + \frac{\hbar^2}{24} \frac{d+4}{d} n T \Delta \ln n \right) \\
&\quad - \frac{d+4}{2} n T \nabla V_B[n] - \left( \frac{d+2}{2} n T + \frac{\hbar^2}{12d} n \Delta \ln n \right) \nabla V \\
&\quad + \frac{\hbar^2}{12} n (\nabla \nabla \ln n) \nabla V + \frac{\hbar^2}{8} \nabla \Delta \ln n.
\end{aligned} \tag{261}$$

The derivation of these relations is beyond the scope of this review and we refer the reader to [23]. It is also unknown if this model possesses a strictly decaying entropy. Indeed, there is no reason why the expansion up to order  $O(\hbar^2)$  of the quantum entropy of the Energy-Transport model would be time decaying. This property has not been proved right nor wrong.

We close this section about Quantum Energy-Transport models by a few remarks. The first one is that there is no rigorous proof neither for the existence of solutions nor for its derivation from the collisional Wigner equation. Numerical simulations have not been performed yet either. In the literature, quantum energy-transport models can be found but their derivation (and the model itself) are different. For instance, we refer to the energy-transport extension of the DG (Density-Gradient) model by Chen and Liu [19].

## 4.2 Quantum Drift-Diffusion model

This section summarizes a series of works [23], [24], [32], [21].

In the classical setting, the Drift-Diffusion model is a simplification of the Energy-Transport model when the assumption of constant temperature is made. To derive a Quantum-Drift-Diffusion model, we start by a discussion of the appropriate BGK operator.

This operator will be defined as a relaxation to a quantum Maxwellian with a fixed temperature, and can be expressed by

$$Q(w)(v) = -\nu(w - \mathcal{E}xp(A - |p|^2/2)), \quad (262)$$

where the function  $A(x)$  is such that the operator conserves mass. Here again, we take a constant temperature equal to unity for the sake of simplicity.

For a given density  $n(x)$ , the Quantum Maxwellian which has density  $n$  in Wigner form is given by

$$\mathcal{M}_n = \mathcal{E}xp(A - |p|^2/2), \quad (263)$$

$$\int \mathcal{E}xp(A - |p|^2/2) \widetilde{dp} = n. \quad (264)$$

In density operator form it is written

$$\rho_n = W^{-1}(\mathcal{M}_n) = \exp(W^{-1}(A - |p|^2/2)), \quad (265)$$

with, for all test function  $\phi$ :

$$\text{Tr}\{\rho_n \phi\} = \int n\phi dx. \quad (266)$$

This Quantum Maxwellian satisfies the free energy minimization principle:  $\rho_n = \exp(W^{-1}(A - |p|^2/2))$  is a solution of the problem: to find

$\min \{G[\rho] = \text{Tr}\{\rho(\ln \rho - 1) + \mathcal{H}\rho\}$  subject to:

$$\text{Tr}\{\rho_n \phi\} = \int n\phi dx, \quad \forall \text{ test fct } \phi \quad \}, \quad (267)$$

where  $\mathcal{H} = |p|^2/2 + V$  is the system Hamiltonian.

In Wigner form, the free energy is written

$$G[\rho] = \text{Tr}\{\rho(\ln \rho - 1) + \mathcal{H}\rho\} = \int [w(\mathcal{L}n w - 1) + \mathcal{H}w] dx \widetilde{dp}, \quad (268)$$

with the quantum logarithm  $\mathcal{L}n w = W[\ln(W^{-1}(w))]$ .

For a given Wigner distribution  $w$ , we denote  $\mathcal{M}_w := \mathcal{M}_n$  the Quantum Maxwellian which has the same density  $n$  as  $w$ :

$$\int \mathcal{M}_w dp = \int w dp. \quad (269)$$

Then Quantum BGK operator is finally written

$$Q(w) = -\nu(w - \mathcal{M}_w). \quad (270)$$

In density operator formulation, we denote by  $\mathcal{M}_\rho$  the Quantum Maxwellian associated with  $\rho$ , and the BGK operator is written:

$$\mathcal{Q}(\rho) = -\nu(\rho - \mathcal{M}_\rho). \quad (271)$$

The situation modeled by  $Q(w)$  is that of a system where energy exchanges between the particles and the surrounding relax the temperature to the background temperature.

Again, two variables appear, the conservative variable  $n$  and the entropic variable  $A$ , with a functional change of variable between these two variables which can be expressed through the free energy and its Legendre dual.

We now list the properties of  $Q$

(i) Mass conservation:

$$\int Q(w) dp = 0, \quad (272)$$

(ii) Null set of  $Q$  (equilibria) :

$$Q(w) = 0 \iff \exists A \text{ such that } w = \mathcal{E}xp(A - |p|^2/2), \quad (273)$$

(iii) Free energy decay:

$$\int Q(w)(\mathcal{L}nw + \mathcal{H}) dx \widetilde{dp} = \text{Tr}\{\mathcal{Q}(\rho)(\ln \rho + \mathcal{H})\} \leq 0. \quad (274)$$

The proof of (iii) is similar to the energy-transport case and is omitted. We now look at the Wigner equation under diffusion scaling:

$$\eta^2 \frac{\partial w^\eta}{\partial t} + \eta(v \cdot \nabla_x w^\eta - \Theta(w^\eta)) = Q(w^\eta), \quad (275)$$

The limit  $\eta \rightarrow 0$  leads to the Quantum Drift-Diffusion model: more precisely, as  $\eta \rightarrow 0$ ,  $w^\eta \rightarrow \mathcal{E}xp(A - |p|^2/2)$  where  $A$  satisfies the Energy-Transport model which consists of the mass conservation equation

$$\frac{\partial n}{\partial t} + \nabla_x \cdot j_n = 0. \quad (276)$$

with

$$\int \mathcal{E}xp(A - |p|^2/2) \widetilde{dp} = n, \quad (277)$$

and the flux  $j_n$  given by

$$j_n = -\nu^{-1}[\nabla \Pi + n \nabla V], \quad (278)$$

with

$$\Pi(A) = \int \mathcal{E}xp(A - |p|^2/2) p \otimes p \widetilde{dp}. \quad (279)$$

The derivation of this model from the collisional Wigner equation follows exactly the same lines as in the Energy-Transport case and is omitted.

Now, the fluid free energy is the kinetic free energy evaluated on the equilibrium  $\mathcal{G}(n) = G(\mathcal{M}_n)$  and is given by

$$\begin{aligned} \mathcal{G}(n) &= \int \mathcal{M}_{n,\mathcal{W}} (\mathcal{L}_n \mathcal{M}_{n,\mathcal{W}} - 1 + \mathcal{H}) dx \widetilde{dp} \\ &= \int \mathcal{E} \exp(A - |p|^2/2) (A - |p|^2/2 - 1 + \mathcal{H}) dx \widetilde{dp} \\ &= \int n(A + V - 1) dx. \end{aligned} \quad (280)$$

Then if either  $V$  is independent of  $t$  or  $V$  is given by Poisson's equation

$$\Delta V = n, \quad (281)$$

then

$$\frac{d}{dt} \mathcal{G}(n) \leq 0, \quad (282)$$

(in the latter case, we have to multiply the term  $nV$  by a factor  $1/2$ ).

We now give a more tractable expression of the pressure tensor  $\Pi$  than (279). We just remark that  $\Pi(A) = \Pi(-A, 0)$  where  $\Pi(A, B)$  is the pressure tensor of the Isentropic Quantum Euler model:

$$\Pi(A, B) = \int \mathcal{E} \exp(-H(A, B)) p \otimes p \widetilde{dp}, \quad (283)$$

with  $H(A, B) = |p|^2/2 - B \cdot p + A + |B|^2/2$ . In that case, we proved (see section 3.3) that

$$\nabla \Pi(A, B) = \nabla(nu \otimes B) + (\nabla B)nu - n\nabla(A + |B|^2/2). \quad (284)$$

In the present case here,  $\nabla \Pi(A)$  is deduced through the identification  $B = 0$  and  $A \rightarrow -A$  which leads to

$$\nabla \Pi(A) = n\nabla A. \quad (285)$$

This leads to an equivalent formulation of the QDD model:

$$\frac{\partial n}{\partial t} + \nabla_x \cdot j_n = 0, \quad (286)$$

$$j_n = -\nu^{-1}(n\nabla(A + V)), \quad (287)$$

$$\int \mathcal{E} \exp(A - |p|^2/2) \widetilde{dp} = n. \quad (288)$$

The moment reconstruction problem (288) has also a simpler expression if we suppose that the Hamiltonian  $H(A) = |p|^2/2 - A$  has a discrete spectrum with eigenvalues  $\lambda_p(A)$  and eigenfunctions  $\psi_p(A)$ ,  $p = 1, \dots, \infty$ . Following (145), we have

$$n(A)(x) = \sum_{p=1}^{\infty} \exp(-\lambda_p(A)) |\psi_p(A)(x)|^2. \quad (289)$$

The 'final' expression of the Quantum Drift-Diffusion model is therefore:

$$\frac{\partial n}{\partial t} + \nabla_x \cdot j_n = 0, \quad (290)$$

$$j_n = -\nu^{-1}(n\nabla(A+V)), \quad (291)$$

$$n(A)(x) = \sum_{p=1}^{\infty} \exp(-\lambda_p(A)) |\psi_p(A)(x)|^2. \quad (292)$$

with  $\lambda_p(A)$  and  $\psi_p(A)$  the eigenvalues and eigenvectors associated with the modified Hamiltonian  $H(A) = |p|^2/2 - A$ .

Now, we would like to consider the equilibrium states of the QDD model, defined by  $j_n = 0$ . This obviously implies  $A = -V$  (up to a constant that we take equal to zero). Therefore, the moment reconstruction problem becomes

$$n(x) = \sum_{p=1}^{\infty} \exp(-\lambda_p) |\psi_p(x)|^2, \quad (293)$$

with  $\lambda_p, \psi_p$  the eigenvalue and eigenvector associated with the 'true' system Hamiltonian  $H(-V) = |p|^2/2 + V$ . If additionally,  $n$  is related with  $V$  through Poisson's equation (281), this leads to the well-known Schrödinger-Poisson problem which characterizes equilibrium states.

Now, if we assume that we are close to equilibrium, we can make the approximation  $A \approx -V$  and replace  $A$  by  $-V$  in the moment reconstruction problem (288), which leads to the following system

$$\frac{\partial n}{\partial t} + \nabla_x \cdot j_n = 0, \quad (294)$$

$$j_n = \nu^{-1}(n\nabla(A+V)), \quad (295)$$

$$n(A)(x) = \sum_{p=1}^{\infty} \exp(A+V-\lambda_p(-V)) |\psi_p(-V)(x)|^2, \quad (296)$$

in which case, the spectral problem to be solved is associated with the 'true' system Hamiltonian  $H(-V) = |p|^2/2 + V$ . This system is known as the Schrödinger-Poisson-Drift-Diffusion and has been investigated by Sacco and coauthors in [27, 51, 58].

We now investigate  $\hbar$  expansions of the QDD model. Up to  $O(\hbar^2)$  terms, the QDD model reads:

$$\partial_t n + \nabla \cdot j_n = 0, \quad (297)$$

$$j_n = -\nu^{-1}[\nabla n - n\nabla(V+V_B[n])], \quad (298)$$

$$V_B[n] = -\frac{\hbar^2}{6} \frac{1}{\sqrt{n}} \Delta(\sqrt{n}). \quad (299)$$

This model is called the Density-Gradient model and has first been proposed by Ancona and coauthors [1, 2, 3]. We note that this is just the classical drift-diffusion model with the addition of the Bohm potential (divided by a factor 3 as compared with the Bohm potential of the single-particle hydrodynamics). Usually, this factor is treated as a fitting parameter in the simulation codes.

It is a remarkable fact that the Density-Gradient model has an entropy, which is nothing but the free energy of the QDD model expanded up to  $O(\hbar^2)$  terms:

$$\mathcal{G}_2(n) = \int_{\mathbb{R}^d} n(\ln n - 1 + V + V_B[n]) dx. \quad (300)$$

If  $V$  is independent of  $t$  it can be shown that

$$\frac{d}{dt}\mathcal{G}_2(n) = - \int_{\mathbb{R}^d} \frac{1}{\nu n} |\nabla n + n\nabla(V + V_B[n])|^2 dx \leq 0. \quad (301)$$

A similar expression would hold if  $V$  is solved through Poisson's equation (281). The proof can be found in [23].

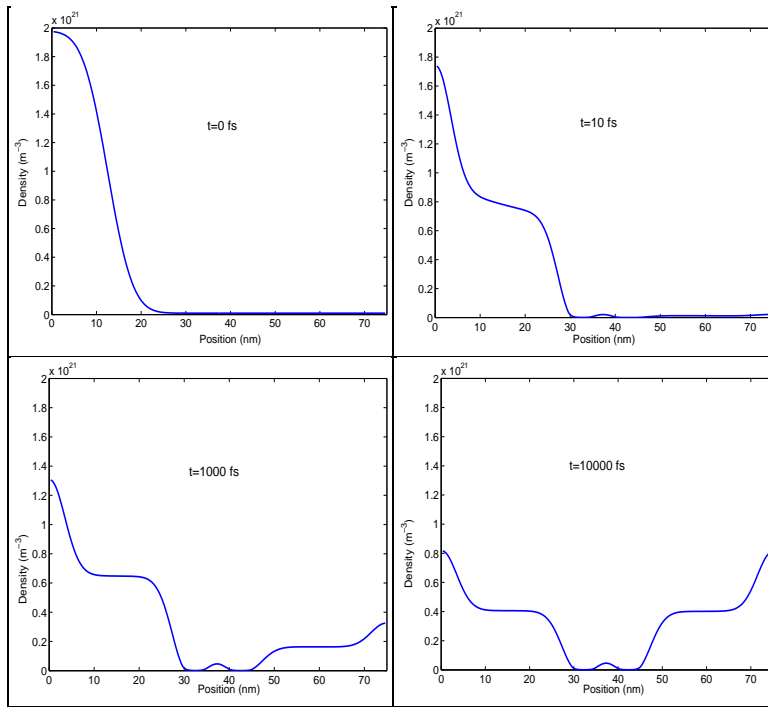
The Density-Gradient model has been widely investigated in the literature. The mathematical theory has been settled first by Ben Abdallah and Unterreiter in [11] and later by Pinnau [56]. Numerical methods have been developed by Pinnau and Unterreiter [57] and Jüngel and Pinnau [42]. The present approach provides a derivation of the DG model from first principles and proves (for the first time) that DG model is compatible with free energy decay.

About the full QDD model (i.e. with no  $\hbar$  expansion), there is no rigorous proof, neither of existence nor of convergence.

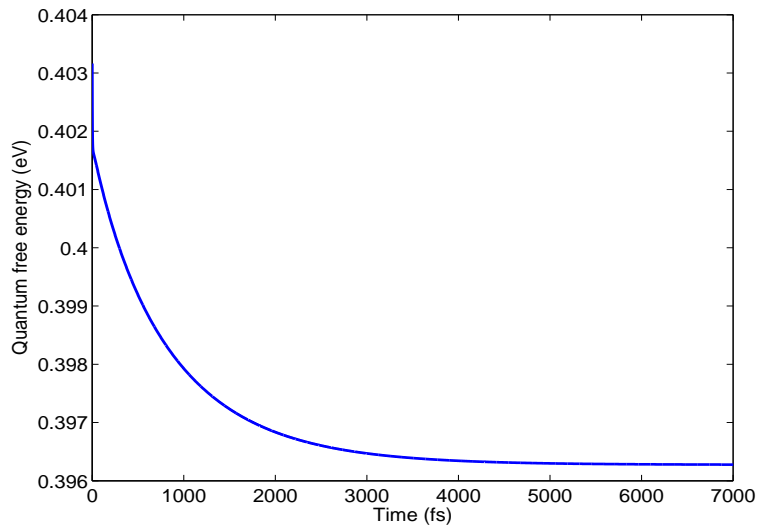
We now present some numerical simulations. We first show a Resonant Tunneling Diode with insulating boundary conditions. The parameters are all chosen independent of  $x$  in this case and are given in table 2. The initial density is concentrated to the left of the double barrier and figure 6 shows the evolution of electrons for the QDD model coupled with Poisson equation under insulating boundary conditions. The next figure (figure 7) demonstrates that the quantum free energy is a decreasing function of time. Figure 8 displays the evolution of the electrochemical potential  $\varphi(x) = A(x) - V(x)$ .

effect. mass( $kg$ )	mobility ( $m^2V^{-1}s^{-1}$ )	permittivity ( $Fm^{-1}$ )	temperature (K)
$0.067 \times 9.11e - 31$	0.85	$11.44 \times 8.85e - 12$	300

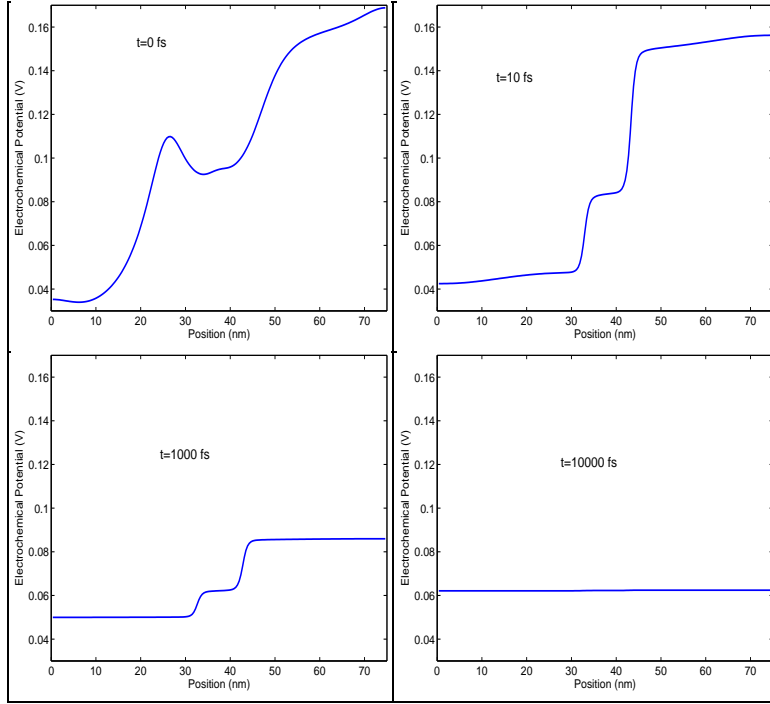
**Table 2.** Parameters used for the modeling of an isolated RTD.



**Fig. 6.** Electron density at different times ( $t = 0, 10, 1000$  and  $10000$  fs) for the QDD model.



**Fig. 7.** Evolution of the Quantum free energy.

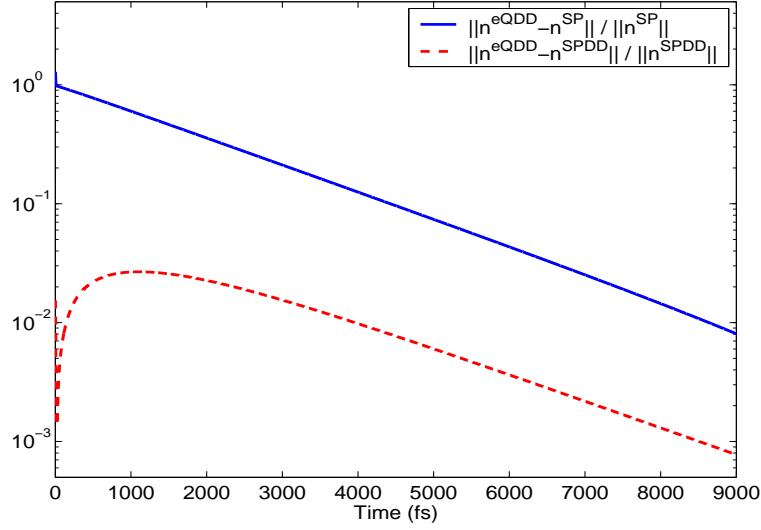


**Fig. 8.** Electrochemical potential ( $\varphi(x) = A - (V_s + V_{ext})$ ) at different times ( $t = 0, 10, 1000$  and  $10000$  fs).

Figure 9 permits to compare the QDD model, the Schrödinger-Poisson-Drift-Diffusion (SPDD) model and the stationary Schrödinger-Poisson (SP) model. The QDD and the SPDD model are closer than the QDD and the SP models.

Now, we look at open boundary conditions. We first analyze the influence of the effective mass on the shape of the current-voltage characteristic. The temperature is chosen equal to  $77K$  and the mobility is supposed to be constant and equal to  $0.85 \text{ m}^2\text{V}^{-1}\text{s}^{-1}$ . The permittivity is also supposed to be constant and equal to  $11.44 \epsilon_0$ . Figure 10 shows four different IV curves with different values of the effective mass inside and outside the double barriers. These curves show a certain sensitivity of the model to the value of the effective mass inside the barrier.

Figure 11 shows the time evolution of the density from the peak to the valley when the effective mass is  $m_2 = 1.5 \times 0.092m_e$  inside the barriers and  $m_1 = 1.5 \times 0.067m_e$  outside it (corresponding to the IV curve at the bottom right of figure 10). To obtain this figure, we apply a voltage of  $0.25V$  and wait



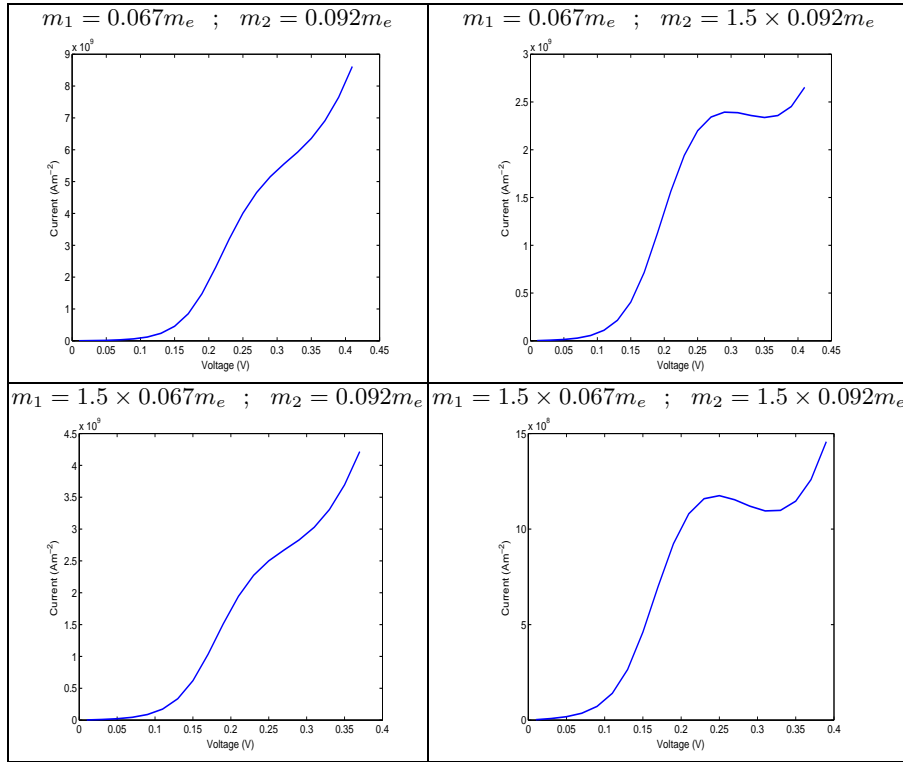
**Fig. 9.** Comparison between the QDD model and the SPDD model (dashed line), and between the QDD model and the SP model (solid line).

for the electrons to achieve the stationary state. Then we suddenly change the value of the applied bias to  $0.29V$  and we record the evolution of the density. As expected, the density inside the well grows significantly and the stationary state is achieved at about  $1500fs$ .

The next two figures (fig. 12 and fig. 13) display the details of the reconstruction of the density from the eigenstates  $\psi_p$  (for  $p = 1 \dots 6$ ) of the modified Hamiltonian  $H[A]$ . The density  $e^{-\lambda_p}|\psi_p|^2$  corresponding to each eigenstate is plotted for two values of the applied bias, respectively corresponding to the current peak (fig.12) and to the valley (fig.13). Table 4.2 shows the values of the corresponding energies  $\lambda_p$ . Last, figure 14 shows the transient current at the left contact ( $x = 0$ ). A detailed discussion of these results can be found in [21]

	$\lambda_1$	$\lambda_2$	$\lambda_3$	$\lambda_4$	$\lambda_5$	$\lambda_6$	$\lambda_7$
Peak	0.87	1.05	1.56	2.03	2.28	3.03	4.47
Valley	0.87	1.11	1.57	1.70	2.54	3.05	5.03

**Table 3.** Eigenvalues (Energies [eV]) of the modified Hamiltonian  $H[A]$  at the Peak and at the Valley.

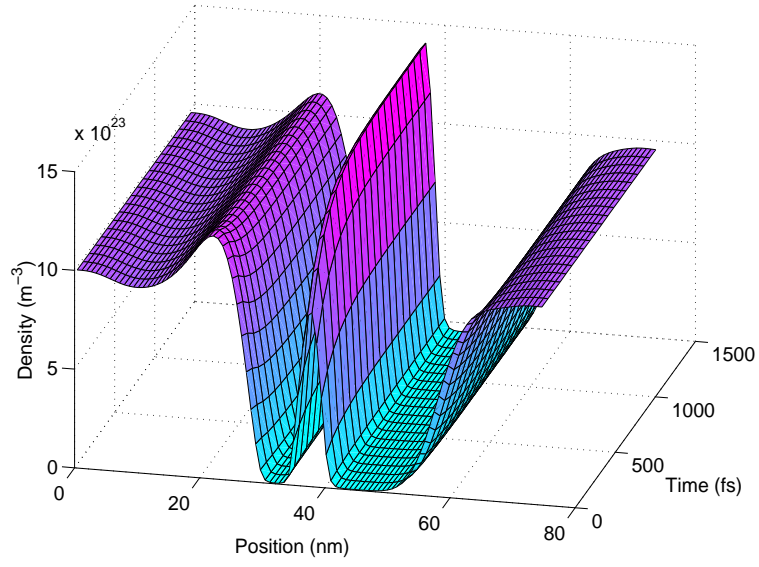


**Fig. 10.** Influence of the effective mass on the IV curve,  $m_1$  being the mass outside the barriers, and  $m_2$  being the mass inside.

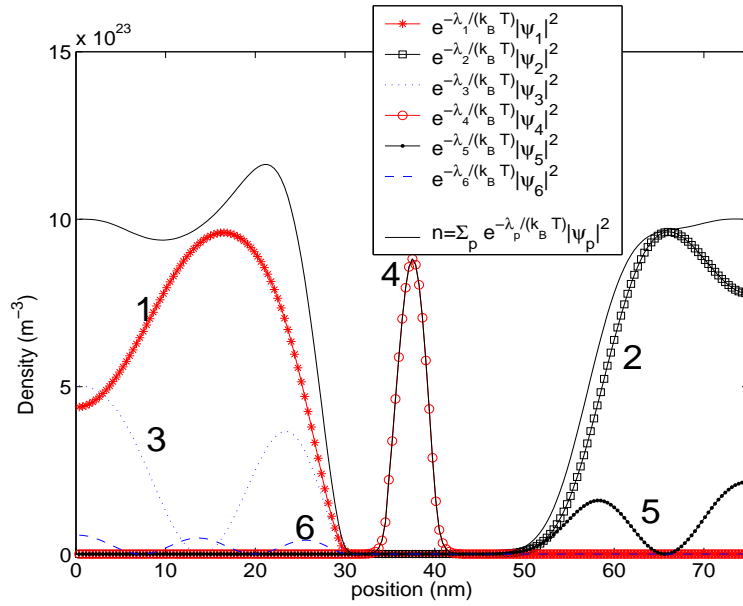
In Figure 15, we show the results obtained with the Density Gradient model using the same parameters as defined for the QDD model. As we can see, results are qualitatively similar but differ significantly. Even with a smoother external potential (replacing the two step functions by two gaussians), it appears that the current-voltage characteristics are still different for the two models as suggested by figure 16. To finish, figure 17 shows the role of the temperature on the current for an applied bias of  $0.2V$  and for the three models QDD, DG and CDD with a constant mass equal to  $0.067m_e$ .

### 5 Summary and conclusion

In these lecture notes, after reviewing the basics of quantum statistical mechanics of nonequilibrium systems (density operator, quantum Liouville equa-



**Fig. 11.** Evolution of the density from the peak (applied bias: 0.25V) to the valley (applied bias: 0.31V).



**Fig. 12.** Density at the peak (Applied bias: 0.25V).

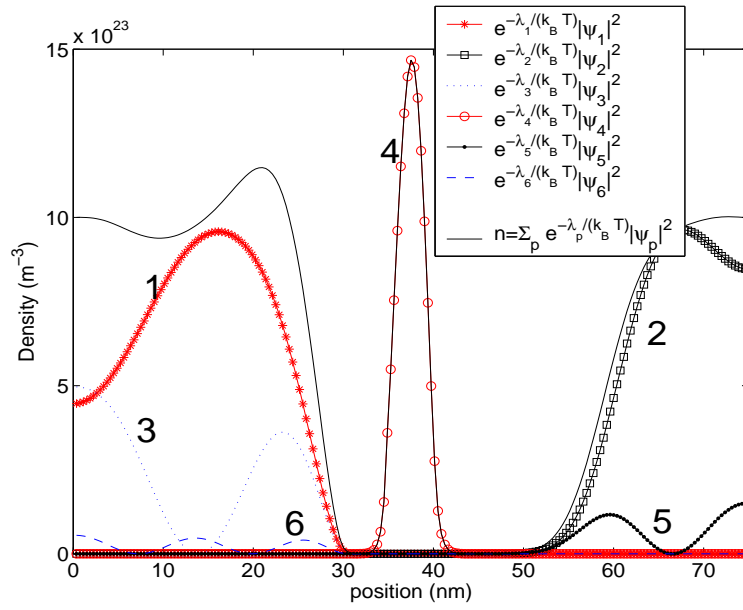


Fig. 13. Density at the valley (Applied bias: 0.31V).

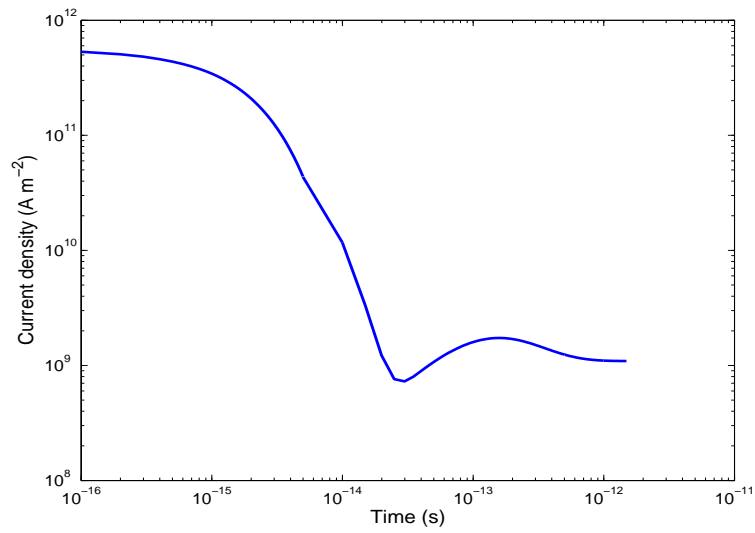
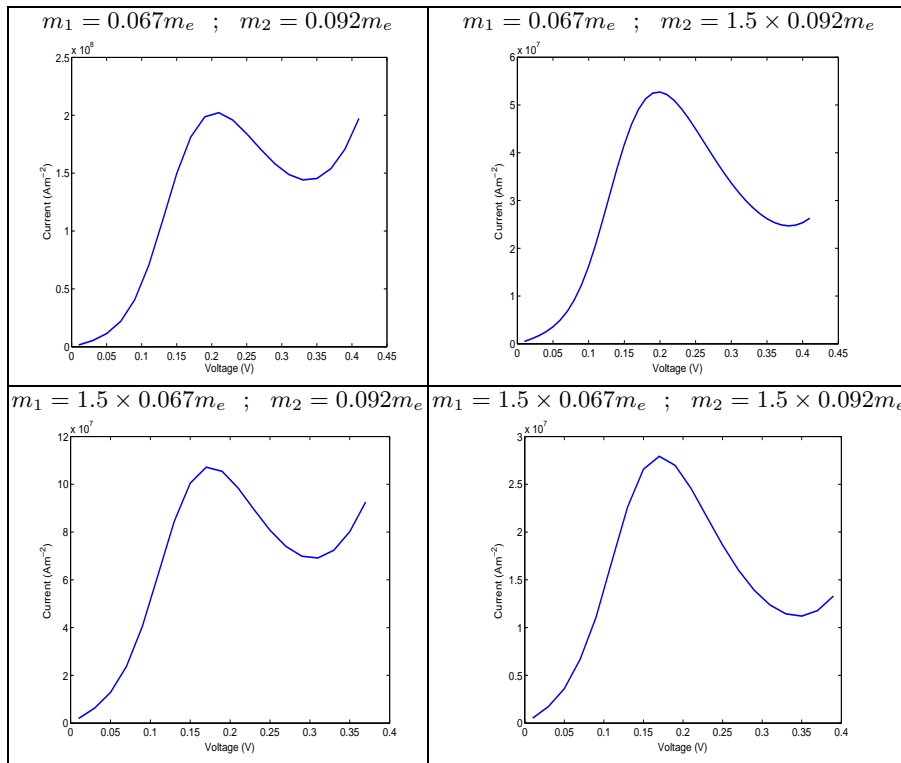


Fig. 14. Transient Current density.

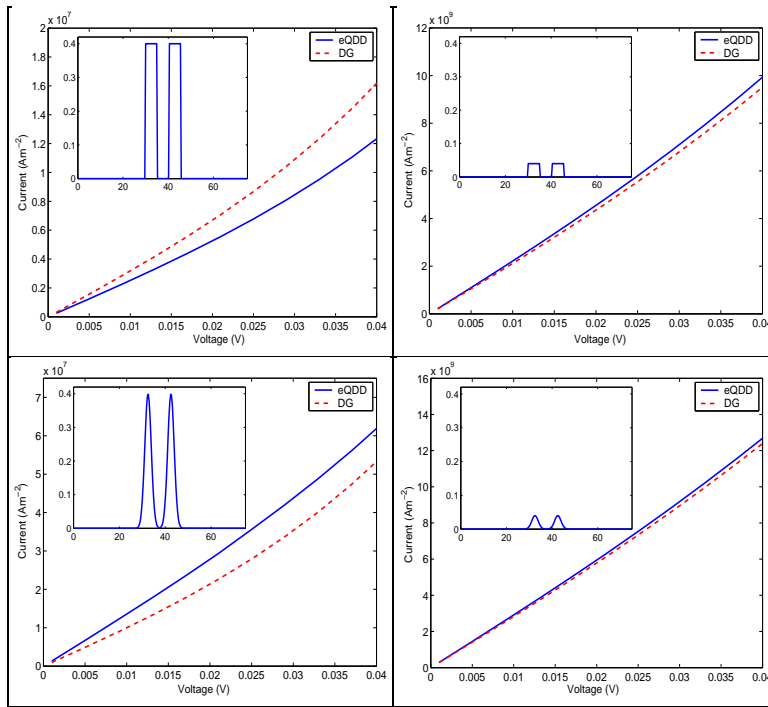


**Fig. 15.** IV curves obtained with the DG model ( $m_1$  being the mass outside the barriers, and  $m_2$  being the mass inside).

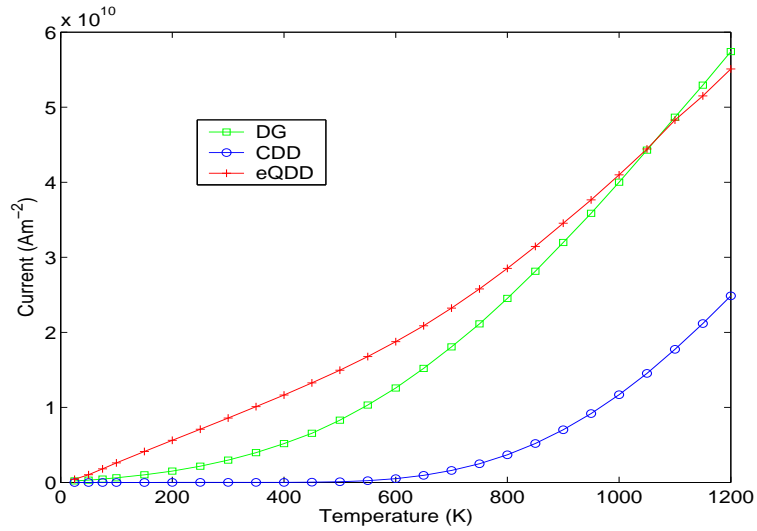
tion, Wigner transform and Wigner equation, mean-field limits, Hartree and Hartree-Fock systems), we have discussed the modeling of open systems interacting with a large and imperfectly known environment and have briefly summarized previous quantum hydrodynamic approaches.

Then, we have developed our approach for deriving new quantum hydrodynamic systems based on the entropy minimization principle. This approach relies on a suitable extension of Levermore's moment method to the quantum case. It consists in taking local moments of the density operator equation and closing the resulting chain of equations by a minimizer of the entropy functional subject to moment constraints. It leads to a formulation of the entropy minimization problem as a global problem (whereas it is a local problem in classical mechanics) and results in a non-local closure of the so-obtained Quantum Hydrodynamic equations.

Then, we have considered the special case of the Isothermal Quantum Euler model, which is the quantum hydrodynamic model corresponding to the isothermal Euler system in classical mechanics. In this case, since the temperature is a constant, the role of the entropy is played by the free energy.



**Fig. 16.** Influence of the shape and the height of the double barrier on the Current-Voltage characteristics for the QDD and DG models.



**Fig. 17.** Current-Temperature curve (applied bias: 0.2V).

Analytic computation of the expression of the pressure tensor were possible in terms of both the conservative variables  $(n, nu)$  and the entropic ones  $(A, B)$ . The two systems are related one to each other by the free energy and its Legendre dual. A remarkable gauge invariance property for this system has been exhibited. As a by-product, a constraint between the velocity  $u$  and its adjoint entropic variable  $B$  has been discovered. Several equivalent formulations of the model are possible. Irrotational flows present a special interest, since in this case,  $u = B$  and the problem depends on  $A$  only, which reduces the size of the moment reconstruction problem (i.e. the inversion of the mapping  $A \rightarrow n$ ). A particular interesting case of irrotational flows are one-dimensional flows. Preliminary numerical simulations seem to indicate that the model gives meaningful results in realistic situations.

Many open problems do remain. The most formidable one is obviously to show that the entropy minimization problem has a solution in a reasonable sense. An analytical computation of the closure relations in the case of the full QHD model (as done for the isothermal case) is certainly at reach. The investigation of gauge invariance properties for the full QHD problem is of course mandatory. Another interesting problem is the investigation of the small  $T$  asymptotics (which has formally been realized for the isothermal case in [22]). The  $\hbar$  expansion up to order  $\hbar^2$  is available in [22] or in the work of Jüngel, Matthes, Milisic [41]). Finally, a normal mode analysis of the linearized model would at least give some indication about the well-posedness of the model.

In a last section, diffusion models have been derived by means of the same approach. We have first proposed a formulation of a quantum BGK operator (which models a relaxation of the Wigner distribution function towards a quantum equilibrium). Then, we have performed a diffusion approximation of the resulting Quantum Kinetic Equation and provided new Quantum Energy-Transport or Drift-Diffusion models. The Quantum Drift-Diffusion model has been analyzed in more detail. This model differs from classical models by the reconstruction of the density from the chemical potential (through an eigenvalue problem). We can recover the Density-Gradient (DG) model of Ancona, and Iafrate [2] as an  $O(\hbar^2)$  approximation, and the Schrödinger-Poisson Drift-Diffusion (SPDD) model of Sacco et al [27] in situations close to equilibrium. A large set of numerical simulations have been realized and show that the qualitative behaviour of the model is fairly satisfactory, while a certain sensitivity to some physical parameters still needs to be understood.

The quantum Energy-Transport model needs to be analyzed in the same way. The first step would be to find a simplified expression of the model (having local values of the pressure tensors in terms of the conservative and entropic variables).

Multi-Dimensional simulations will require more computing power but are within reach. A better account of the continuous spectrum of the operators would certainly improve the results, notably close to the boundaries.

Of the overall approach, some other extensions and applications will require further developments. One would wish to introduce many particle effects more accurately than through the use of the BGK collision operator. Using this approach, phonon-electron collision operators for electrons in crystals could be derived. Also, the introduction of confinement in one or more directions would lead to sub-band models which could be applied to systems such as quantum wires or quantum dots. Following the same lines, Born-Oppenheimer approximations in quantum chemistry could also be used in the framework in these models and would lead to hybrid quantum-classical models, in the spirit of [17]. Applications could span from reaction dynamics in chemistry to biology problems such as ionic channels in cell membrane physiology.

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