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Quantum Moment Hydrodynamics and the Entropy Principle

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This paper presents how a non-commutative version of the entropy extremalization principle allows to construct new quantum hydrodynamic models. Our starting point is the moment method, which consists in integrating the quantum Liouville equation with respect to momentum p against a given vector of monomials of p. Like in the classical case, the so-obtained moment system is not closed. Inspired from Levermore's procedure in the classical case,[26] we propose to close the moment system by a quantum (Wigner) distribution function which minimizes the entropy subject to the constraint that its moments are given. In contrast to the classical case, the quantum entropy is defined globally (and not locally) as the trace of an operator. Therefore, the relation between the moments and the Lagrange multipliers of the constrained entropy minimization problem becomes nonlocal and the resulting moment system involves nonlocal operators (instead of purely local ones in the classical case). In the present paper, we discuss some practical aspects and consequences of this nonlocal feature.

KEY WORDS: Density matrix; quantum entropy; quantum moments; local quantum equilibria; quantum BGK models; quantum hydrodynamics.

1. INTRODUCTION

The aim of this paper is to present a new approach to quantum hydrodynamics. More precisely, starting from the quantum Liouville equation, we derive a whole hierarchy of moment models including quantum hydrodynamical models as well as higher order moment models. The so-obtained models will be referred to as "Quantum Moment Hydrodynamics."

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The derivation of quantum hydrodynamic models from first principles has attracted considerable attention in the recent past. The quest for such models is driven by the growing field of nanotechnology applications. The derivation of reliable yet computationally affordable many-particle quantum models determines the possibility of efficient industrial design and fabrication of the next generation of devices. However, few attempts have been successful in this direction. Indeed, away from the complete resolution of the Schrödinger equation (or even worse, of the quantum Liouville equation), which is computationally expensive, and the use of continuum models with ad-hoc phenomenological closure and limited reliability, few alternatives are available. The starting point for the derivation of quantum hydrodynamic models is the quantum Boltzmann equation of the form

$$i\hbar\,\partial_t \rho = [H, \rho] + Q(\rho), \tag{1.1}$$

for the effective single particle density matrix $\rho(x, y)$, where H is the Hamiltonian $H = -\frac{\hbar^2}{2m^*}|\nabla_x|^2 + V(x)$, the symbol $[\cdot, \cdot]$ denotes the usual commutator and the operator Q models particle collisions. $\hbar$ denotes the reduced Planck constant and m^* is the particle (effective) mass. To derive fluid like models for macroscopic quantities it is convenient to consider instead the equivalent formulation via Wigner functions, which is of the form

$$\partial_t f_w + \mathrm{div}_x\left(\frac{1}{m^*} p f_w\right) - \theta[V]\, f_w = Q_w(f_w), \tag{1.2}$$

where the Wigner function $f_w(x, p, t)$ and the pseudo-differential operator θ are related to the density matrix ρ and the potential V via the Wigner transform

$$\begin{aligned} f_w(x, p, t) &= (2\pi)^{-d} \int_{\mathbb{R}^d} \rho\left(x - \frac{\hbar}{2}\eta, x + \frac{\hbar}{2}\eta\right) e^{i\eta\cdot p}\, d\eta, \\ \theta[V] &= \frac{i}{\hbar}\left[V\left(x + \frac{\hbar}{2i}\nabla_p\right) - V\left(x - \frac{\hbar}{2i}\nabla_p\right)\right] \end{aligned} \tag{1.3}$$

where $\rho(x, y)$ is the integral kernel of ρ and d is the space dimension (an integer multiple of 3 according to the number of degrees of freedom). Moment systems for the Wigner–Boltzmann equation (1.2) are equations for a given set of moments

$$m_n(x, t) = \int_{\mathbb{R}^d} \kappa_n(p)\, f_w(x, p, t)\, dp, \qquad n = 0, \ldots, N, \tag{1.4}$$

which are obtained by building the corresponding moments of (1.2). The main problem in closing this system, i.e., expressing the highest order moments in the resulting equations in terms of the lower order moments, is that the collision operator Q (or Q_w in (1.2)) is not available in a sufficiently simple form, to be used in a Chapman–Enskog-like approach to moment closures. Collision operators for scattering with phonons on the weak coupling limit have been derived and analyzed in refs. 2, 5, 12 and quantum versions of Fokker–Planck type operators have been derived in refs. 3 and 6.

First attempts towards the derivation of quantum hydrodynamic models have used BKW waves. Writing the wave-function as $\psi = \sqrt{n(x, t)} \times \exp(iS(x, t))$, where n is the probability of presence and S is the phase and inserting it into the Schrödinger equation gives rise to a set of two equations for n and $n \nabla S$ which mimic the clasical density and momentum conservation equations. Compared with the classical case, the momentum equation involves an additional term, called the Bohm potential. This approach has been investigated in refs. 16, 17, 20, and 23. This is however a pure-state model which does not incorporate mutli-particle effects and which can be viewed as a zero-temperature model. Finite temperature effects have been taken into account in ref. 18 through the use of a nonlinear Schrödinger equation and gives rise to a momentum equation with a nonlinear enthalpy relation. The equation-of-state is local (i.e., the pressure (or the enthalpy) depends locally on the density at the same point). In ref. 22, it is argued that the Bohm potential approach is not consistent with the entropy condition. The approach presented in this paper brings a cure to this problem.

Other approaches[11, 13] make use of moment closures of the Wigner equation using semiclassical asymptotics (i.e., a limit $\hbar \to 0$ where $\hbar$ is the Planck constant) for thermodynamical equilibrium states as closures. They give rise to local equations-of-state as well, which coincide with the previous theories up to constant factors. Related to this approach are moment closure theories of the Wigner equation using small-field asymptotics for thermodynamical equilibria.[14, 15] These give rise to nonlocal equations-of-state. However, the nonlocality enters only through the potential.

The idea behind the work presented in this paper is to use a thermodynamic approach using the minimal amount of information about the collision operator necessary to derive moment equations. That is we assume knowledge about the corresponding moments of the collision operator and the existence of an entropy which is dissipated by the collisions. Our approach bears strong similarities with the theory of NESOM (for Non-Equilibrium Statistical Operator Mechanics) by Zubarev and coworkers[28, 36] (see also the review paper by Luzzi[27]). However, we give

a neater (and to some extent, more practical) mathematical framework which, we believe, will be useful for further developments of the theory. We shall elaborate more on the relation between our theory and NESOM in Section 4, Remark 4.2.

Our approach consists in taking moments of the density matrix equation (or quantum Liouville equation), and then, closing the resulting set of moment equations with an equilibrium density matrix. This equilibrium is found as an extremum of the entropy functional subject to the constraints that its moments coincide with those of the density matrix we are considering. This approach is therefore similar to Levermore's closure moment hierarchies[26] or to the extended thermodynamics approach[29] for classical systems

To be more, specific, let a set of polynomials $\kappa(p) = (\kappa_0(p),..., \kappa_N(p))$ be given. To any ρ, we associate a set of moments $m[\rho] = (m_0(x),..., m_N(x))$ defined by duality as the representation of the linear functionals $\lambda \to \mathrm{Tr}\{\rho\ \mathrm{Op}(\lambda \cdot \kappa)\}$, where $\lambda = (\lambda_0(x),..., \lambda_N(x))$, $\lambda \cdot \kappa = \sum_i \lambda_i(x)\, \kappa_i(p)$ and Op means the Weyl quantization of a symbol (i.e., a function of position x and momentum p) into an operator. This definition of moments by duality will prove more convenient in connection with the entropy minimization principle. If the chosen set of polynomials is equal to $(1, p, |p|^2/2m^*)$, the associated moments correspond to the usual hydrodynamic quantities, i.e., local density, momentum and energy (per particle). If a larger set is chosen, the associated moments correspond to higher order hydrodynamic quantities like the pressure tensor, heat flux vector, higher order heat flux tensor, etc., according to the terminology of extended thermodynamics.[29] For instance, the pressure tensor will be associated with the monomials $p_i\, p_j$ where p_i and p_j denote the components of the momentum vector in the ith and jth direction, respectively.

Now, we turn to the definition of an equilibrium density matrix which satisfies given moment constraints. Such an equilibrium minimizes the entropy (defined as $H(\rho) = \mathrm{Tr}\{h(\rho)\}$ where h is a suitable convex function, like, e.g., the Boltzmann entropy $h(\rho) = \rho(\ln(\rho) - 1)$). In this work, we show that this constrained minimization problem has the solution $\rho^m = (h')^{-1}(\mathrm{Op}(\mu \cdot \kappa))$ where $\mu = (\mu_0(x),..., \mu_N(x))$ are the Lagrange multipliers of the moment constraints $\{m[\rho] = m \text{ given}\}$. $(h')^{-1}$ is the inverse function of the derivative of h. Functions of operators are given a meaning in the sense of functional calculus.

It is now possible to get back to the problem of deriving moment models from the quantum Liouville equation. Taking the moments of the Liouville equation (which is now a precise concept), we can close the chain of moment equations by using the equilibrium just defined. According to the chosen set of polynomials and the number of moments involved, we

obtain a hierarchy of moments systems which we call Quantum Moment Hydrodynamics. We note that such a closure is different from a single-state closure as it takes into account many-particle interactions through the entropy minimization procedure. However, we should recover the single-state closure by a zero-temperature asymptotics (for $\hbar$ being fixed) of our moment models. The investigation of this point is left to future work. Also, the moment systems should obviously constitute an approximation of the original quantum kinetic system (1.1). However, since the expression of $Q(\rho)$ is not known, assessing the accuracy of this approximation is extremely delicate.

The goal of the present paper is to develop these concepts. The paper is organized as follows: in Section 2, we recall Levermore's approach to moment closure hierarchies in the classical case, however giving it a presentation which makes its extension to the quantum case more natural. Then, in Section 3, we extend Levermore's approach to the quantum case, developing our definition of moment. We elaborate more on the fluid entropy and compare our theory with NESOM in Section 4. Quantum moment hydrodynamics systems are derived and studied in Section 5. In particular, it is shown that quantum hydrodynamics for the usual set of moments (density, momentum, and energy) differs from classical hydrodynamics by a possibly non-scalar pressure tensor and nonzero heat flux vector. These are related *nonlocally* to the basic moments through the equilibrium density matrix. Higher order quantum moment systems exhibit similar features. Finally, as noticed in this section, it is possible to make sense to quantum BGK relaxation systems. A conclusion is drawn in Section 6. Finally, technical details are deferred to two appendices (Appendices A and B).

It should be stressed that most of the mathematical properties stated in this paper are given only *formal proofs*. Fully rigorous proofs will require a lot of mathematical developments which are beyond the scope of the present paper. However, a practical usage of these new models does not require that all the mathematical theory is settled. Indeed, this paper should rather be viewed as a presentation of new models and as a programme definition for future work.

The results of the present work have been announced in ref. 9.

2. ENTROPY MINIMIZATION PRINCIPLES AND MOMENT CLOSURE HIERARCHIES IN THE CLASSICAL CASE

In this section, we mainly review the approach proposed by Levermore[26] in the classical case. However, we shall present the entropy minimization principle in a slightly different (but completely equivalent) form which will make it more suitable to an extension to the quantum case.

In classical kinetic theory, the basic object is the particle distribution function $f(x, p, t)$ where $x \in \mathbb{R}^d$ is the position, $p \in \mathbb{R}^d$ is the momentum, and t is the time. f is a probability distribution and is therefore normalized according to

$$\int_{\mathbb{R}^{2d}} f(x, p)\, dx\, dp = 1. \tag{2.1}$$

In all this work, we shall assume that the total number $\mathcal{N}$ of particles in the system is fixed. This hypothesis is not essential in the classical case, but it will greatly simplify the presentation of the quantum case. The distribution function f is a solution of the so-called Boltzmann equation:

$$\frac{\partial f}{\partial t} + \{\hat{H}, f\} = Q(f), \tag{2.2}$$

where $\hat{H}(x, p)$ is the particle Hamiltonian, $\{\hat{H}, f\}$ is the Poisson bracket

$$\{\hat{H}, f\} = \nabla_p \hat{H} \cdot \nabla_x f - \nabla_x \hat{H} \cdot \nabla_p f,$$

and $Q(f)$ is a collision operator, which models the interactions of the particles among themselves or with the surrounding medium.

On the other hand, the physics of continua considers averaged quantities which only depend on the position variable such as the mean density, momentum or energy. These quantities are defined as moments of the distribution function f. More specifically, let $\kappa_i(p)$, $i = 0, \ldots, N$ be $N+1$ independent functions of p and denote by $\kappa(p) = (\kappa_i(p))_{i=0,\ldots,N}$ the vector of monomials. The associated moments $k_i(f)(x)$ of $f(x, p)$ are defined by:

$$k_i(f)(x) = \int_{\mathbb{R}^d} f(x, p)\, \kappa_i(p)\, dp, \qquad \forall x.$$

The equations for $k(f) = (k_i(f))_{i=0,\ldots,N}$ are obtained by multiplying (2.2) by $\kappa_i(p)$ and integrating with respect to p:

$$\frac{\partial k_i(f)}{\partial t} + \int_{\mathbb{R}^d} \kappa_i(p) \{\hat{H}, f\}\, dp = \int_{\mathbb{R}^d} \kappa_i(p)\, Q(f)\, dp. \tag{2.3}$$

In most cases the integrals in (2.3) cannot be expressed in terms of the functions $k_i(f)$ alone. In order to reduce system (2.3) to a closed system for the functions k_i, some assumptions must be made on the distribution function f. According to statistical physics, the most likely distribution function (upon a certain number of realizations) is a minimum of the

entropy functional among functions whose moments are given by the functions k_i. Following ref. 26, we use this Ansatz and replace f in the integrals of (2.3) by this distribution function.

The minimization principle (or Gibbs minimization principle, see ref. 4) can be formulated as follows. Let h be a smooth strictly convex function defined on $[0, \infty)$ and define the entropy functional $H(f)$ acting on functions $f(x, p)$ associated with h by:

$$H(f) = \int_{\mathbb{R}^{2d}} h(f(x, p))\, dx\, dp.$$

Let $m = (m_i(x))_{i=0,\ldots,N}$ be $N+1$ given functions of the position variable x. We are concerned with the following minimization problem (Gibbs problem): find the solution f^m of

$$H(f^m) = \min\{H(f) \mid f \text{ satisfies } k_i(f)(x) = m_i(x), \forall x, \forall i\}. \tag{2.4}$$

The normalization condition (2.1) is not included in the constraints of (2.4). Rather, we assume that the constant function is contained in $\kappa(p)$, say $\kappa_0(p) = 1$. Then, $m_0(x)$ is the probability of presence of a particle in the neighbourhood of x and is such that $\int m_0(x)\, dx = \int f(x, p)\, dx\, dp$. We restrict the set of moments to those satisfying

$$\int_{\mathbb{R}^d} m_0(x)\, dx = 1, \tag{2.5}$$

so that the constraint (2.1) is satisfied, as soon as the constraints of (2.4) are satisfied.

In most physics textbooks, the tradition is to use the opposite sign for the entropy (i.e., to suppose that it is a concave function) and to write the Gibbs principle as a constrained maximization problem. It is the mathematicians' usage however to use the opposite convention. Of course, the two conventions are completely equivalent.

We note that this problem can be equivalently stated as

$$H(f^m) = \min\left\{ H(f) \mid f \text{ satisfies } K_\lambda(f) = \int_{\mathbb{R}^d} m \cdot \lambda\, dx, \right.$$
$$\left. \forall \lambda(x) = (\lambda_i(x))_{i=0,\ldots,N} \right\}, \tag{2.6}$$

where, we have introduced

$$K_\lambda(f) = \int_{\mathbb{R}^d} k(f) \cdot \lambda(x)\, dx = \int_{\mathbb{R}^{2d}} f(x, p)\, \kappa(p) \cdot \lambda(x)\, dx\, dp, \tag{2.7}$$

and, for two vectors a and b of $\mathbb{R}^{N+1}$, we write $a \cdot b = \sum_i a_i b_i$. The arbitrary functions $\lambda = (\lambda_i(x))_{i=0,\ldots,N}$ are the Lagrange multipliers of the constraints.

According to classical optimization theory, the constrained optimization problem (2.4) can be equivalently formulated in terms of a saddle-point problem for the Lagrangian

$$\mathscr{L}_m(f, \lambda) = H(f) - \left(K_\lambda(f) - \int_{\mathbb{R}^d} m(x) \cdot \lambda(x)\, dx \right), \tag{2.8}$$

where the Lagrange multipliers $\lambda = (\lambda_i(x))_{i=0,\ldots,N}$ are functions of x. The saddle-point problem is formulated as follows:

$$H(f^m) = \min_f \max_\lambda \mathscr{L}_m(f, \lambda) = \max_\lambda \min_f \mathscr{L}_m(f, \lambda), \tag{2.9}$$

where now the minimum over f or the maximum over λ are unconstrained problems.

Let us now consider the unconstrained problem

$$\mathscr{L}_m(f_\lambda, \lambda) = \min_f \mathscr{L}_m(f, \lambda). \tag{2.10}$$

Then, the necessary condition for extremality leads to

$$f_\lambda(x, p) = (h')^{-1}(\lambda(x) \cdot \kappa(p)) \tag{2.11}$$

where h' is the derivative of h and $(h')^{-1}$ is the inverse function of h' (which exists since h' is strictly increasing). f_λ is called the equilibrium distribution function and λ is called the system of entropic variables.

Now, the solution f^m of the constrained minimization problem (2.4) is an equilibrium distribution function f_μ where $\mu = \mu^m$ is a solution of the unconstrained maximization problem

$$H(f^m) = \mathscr{L}_m(f_{\mu^m}, \mu^m) = \max_\lambda \mathscr{L}_m(f_\lambda, \lambda). \tag{2.12}$$

The resolution of (2.12) leads to

$$f^m = f_{\mu^m}, \tag{2.13}$$

where μ^m is such that

$$k_i(f_{\mu^m}) = m_i, \qquad \forall i = 1, \ldots, N. \tag{2.14}$$

We note that this relation is equivalent to saying that

$$K_\lambda(f_{\mu^m}) = \int_{\mathbb{R}^d} m(x)\cdot\lambda(x)\,dx, \qquad \forall\lambda(x). \tag{2.15}$$

This last relation is in a form which will be easily extended to the quantum case. The entropic variables μ and the moment (or conservative) variables m are dual (in the Legendre transform sense) through the fluid entropy (see Section 4 where this aspect is developed in the quantum case).

Now, following ref. 26, a closed set of moment equations can be derived from (2.3) by replacing f in the integrals appearing in (2.3) by the solution of the Gibbs principle associated with the constraint that the moments are $k_i(f)$. This leads to a closed system of equations for the moments $m_i = k_i(f)$ which is written as follows:

$$\frac{\partial m_i}{\partial t} + \int_{\mathbb{R}^d} \kappa_i(p)\{\hat{H}, f^m\}\,dp = \int_{\mathbb{R}^d} \kappa_i(p)\,Q(f^m)\,dp. \tag{2.16}$$

For future use, we note that system (2.16) can be written in weak form as:

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^d} m\cdot\lambda\,dx + \int_{\mathbb{R}^{2d}} \lambda(x)\cdot\kappa(p)\{\hat{H}, f^m\}\,dp\,dx$$

$$= \int_{\mathbb{R}^{2d}} \lambda(x)\cdot\kappa(p)\,Q(f^m)\,dp\,dx, \tag{2.17}$$

for all $\lambda(x)$. We shall extend this weak form of the hydrodynamic equations to the quantum case. The key point is to interpret the integrals in (2.17) in an operator way.

We now comment on the form (2.4) of the Gibbs minimization principle. In ref. 26, the Gibbs principle is given a local form. For a function $f(p)$, we denote by $\tilde{H}$ the *"local"* entropy functional

$$\tilde{H}(f) = \int_{\mathbb{R}^d} h(f(p))\,dp.$$

Then, for any given $(N+1)$-tuple of *real numbers* $\tilde{m} = (\tilde{m}_i)_{i=0,\ldots,N}$, the *local Gibbs principle* reads: find $\tilde{f}^{\tilde{m}}(p)$ which realizes

$$\tilde{H}(\tilde{f}^{\tilde{m}}) = \min\{\tilde{H}(f) \mid f(p) \text{ satisfies } K_i(f) = \tilde{m}_i,\ \forall i\}. \tag{2.18}$$

Of course, for $f(x, p)$, we have

$$H(f) = \int_{\mathbb{R}^d} \tilde{H}(f(x, \cdot))\, dx.$$

The solution of the "local" Gibbs minimization principle (2.18) is obviously

$$\tilde{f}^{\tilde{m}} = (h')^{-1}(\tilde{\mu}^{\tilde{m}} \cdot \kappa), \tag{2.19}$$

where $\tilde{\mu}^{\tilde{m}}$ is such that

$$K_i(\tilde{f}^{\tilde{m}}) = \tilde{m}_i, \qquad \forall i. \tag{2.20}$$

This defines a local mapping $\tilde{m} \in \mathbb{R}^{N+1} \to \tilde{\mu}^{\tilde{m}} \in \mathbb{R}^N$. The solution of the global Gibbs principle (2.13) is obviously related to that of the local one (2.19) by:

$$\mu^m(x) = \tilde{\mu}^{m(x)}.$$

However, the global form (2.4) of Gibbs principle can be extended to the quantum case, while the local form cannot. Quantum mechanics is a nonlocal theory and requires that a nonlocal Gibbs principle be used.

Let us review some classical cases. Suppose that the Hamiltonian is given by

$$\hat{H}(x, p) = \varepsilon(p) + V(x, t), \qquad \varepsilon(p) = \frac{|p|^2}{2m^*},$$

where $\varepsilon(p)$ is the kinetic energy, $V(x, t)$, the potential energy and m^* the particle mass. Suppose that the vector κ of monomials is a $d+2$-dimensional vector (d being the dimension of the physical space) consisting of

$$\kappa(p) = (1, (p_i)_{i=1,\ldots,d}, |p|^2/(2m^*)). \tag{2.21}$$

The functions involved in $\kappa(p)$ correspond to the physically conserved quantities (i.e., the probability of presence, the d components of the momentum per particle and the energy per particle). As often in the literature, we shall label the components of this vector according to $\kappa(p) = (\kappa_0(p), (\kappa_i(p))_{i=1,\ldots,d}, \kappa_{d+1}(p))$. In thermodynamics, the associated vector of Lagrange multipliers is usually written

$$\lambda = \left(\frac{\mu_c}{T}, \frac{u}{T}, -\frac{1}{T}\right) := (\lambda_0, (\lambda_i)_{i=1,\ldots,d}, \lambda_{d+1}),$$

where $\mu_c \in \mathbb{R}$ is the chemical potential, $u \in \mathbb{R}^d$ is the mean velocity and $T \in \mathbb{R}^+$ is the temperature. The associated moment vector in turn is written

$$m = (n, q, W) := (m_0, (m_i)_{i=1,\ldots,d}, m_{d+1}),$$

where $n \in \mathbb{R}^+$ is the probability of presence, $q \in \mathbb{R}^d$ is the mean momentum per particle and $W \in \mathbb{R}^+$ is the mean energy per particle. Multiplying n, q, and W by the total number of particles $\mathcal{N}$ gives the number density, the fluid momentum and the fluid energy.

Let us consider specifically the Boltzmann entropy:

$$h(f) = k_B f(\ln f - 1), \tag{2.22}$$

where k_B is the Boltzmann constant. In this case, the equilibrium distribution function f_λ is the classical Maxwellian:

$$\begin{aligned} f_\lambda &= \exp\left\{\frac{1}{k_B}\left(\lambda_0 + \sum_{i=1}^{d} \lambda_i p_i + \lambda_{d+1}\frac{|p|^2}{2m^*}\right)\right\} \\ &= \exp\left\{\frac{1}{k_B T}\left(\mu_c + \sum_{i=1}^{d} u_i p_i - \frac{|p|^2}{2m^*}\right)\right\}. \end{aligned} \tag{2.23}$$

Then, the mapping $m \to \mu^m$ relates (n, q, W) to (μ_c, u, T) in the following way:

$$n = h_P^{-d}\,(2\pi m^* k_B T)^{d/2} \exp\frac{\mu_c + m^*|u|^2/2}{k_B T}, \qquad q = m^* n u,$$

$$W = \frac{1}{2} m^* n\,|u|^2 + \frac{d}{2} n k_B T.$$

With this transformation, the Maxwellian takes the more familiar form

$$f_\lambda = \frac{n}{(2\pi m^* k_B T)^{d/2}} \exp\left\{-\frac{|p - m^* u|^2}{2m^* k_B T}\right\}. \tag{2.24}$$

Supposing that the collision operator is mass, momentum and energy conservative, i.e., satisfies $\int Q(f)\,\kappa_i(p)\,dp = 0$ for all considered κ_i, Eqs. (2.16) can be simplified and gives rise to the usual classical hydrodynamic equations:

$$\frac{\partial n}{\partial t} + \nabla \cdot (nu) = 0, \tag{2.25}$$

$$m^* \left(\frac{\partial nu}{\partial t} + \nabla \cdot (nu \otimes u) \right) + \nabla (nk_B T) = -n \nabla V, \tag{2.26}$$

$$\frac{\partial W}{\partial t} + \nabla \cdot (Wu) + \nabla \cdot (nk_B Tu) = -n \nabla V \cdot u. \tag{2.27}$$

Therefore, the above considered moments give rise to the balance equations for the physically conserved quantities (i.e., mass, momentum and energy).

If other moments than those corresponding to the physically conserved quantities, such as the heat flux (corresponding to $\kappa(p) = p_i |p|^2/2$), the pressure tensor anisotropy (i.e., $\kappa(p) = p_i p_j$), or the higher order heat flux tensor (i.e., $\kappa(p) = p_i p_j p_k$) are considered, new sets of hydrodynamic-like equations are obtained. This gives rise to the so-called "moment closure hierarchies" of Levermore,[26] which are also closely related with the theory of extended thermodynamics.[29] Then, the equilibrium distribution functions (2.11) depend on a larger dimensional vector of Lagrange multipliers λ than the Maxwellians (2.23), which therefore appear as a special case of these equilibria. If one linearizes these equilibria about the Maxwellians (considering that the higher order moments, after convenient normalization, are small), one obtains another moment closure method first proposed by Grad.[19]

However, the following considerations should be borne in mind. First, the N-tuple of monomials $\kappa(p)$ cannot be completely arbitrary. It has to satisfy a certain number of requirements such as gallilean invariance, or the fact that the moments of f_λ must be defined. These constraints are detailed in ref. 26. Second, the existence and uniqueness of solutions of the minimization problems is by far not guaranteed. Moment realizability conditions, i.e., conditions that guarantee that the constrained minimization problem has a solution, as well as uniqueness conditions have been studied in refs. 1, 24, 25, and 32. When moments corresponding to physically non-conserved quantities (i.e., such that the corresponding $\int Q(f)\, \kappa_i(p)\, dp$ is nonzero) are considered, a particular care must be taken in the closure relation for the collision operator part of Eq. (2.3). This must be done in order to capture the correct dynamics in situations which are close perturbations of the usual gas dynamics equations. This point is detailed in ref. 26. Finally, moment systems of the form (2.16) are by construction hyperbolic, which guarantees a certain degree of well-posedness (at least in a linear sense). This point is developed in ref. 26.

We are now going to investigate how these considerations can be extended to the quantum case. For that purpose, we shall use the *nonlocal version* of the Gibbs minimization principle.

3. ENTROPY MINIMIZATION PRINCIPLES IN THE QUANTUM CASE

We first state the entropy minimization principle in the quantum case. To be specific, we consider a system whose objects can be described by wave-functions $\psi(x)$ belonging to the Hilbert space $X = L^2(\mathbb{R}^d)$. In this context, the quantum equivalent of the distribution function is the density matrix ρ which is a positive, trace-class Hermitian operator on X satisfying:[31]

$$\mathrm{Tr}\{\rho\} = 1. \tag{3.1}$$

The normalization condition (3.1) is the quantum counterpart of (2.1). Then, the spectrum of ρ consists of a decreasing sequence of positive eigenvalues $(\alpha_\ell)_{\ell=1,\dots,\infty}$ tending to 0 as $\ell \to \infty$ and the associated eigenvectors ϕ_ℓ constitute a Hilbert basis of X. Moreover, because of (3.1), we have

$$\sum_{\ell=1}^{\infty} \alpha_\ell = 1.$$

The elementary wave-function ϕ_ℓ represents a pure state, while the datum of a density matrix ρ represents a mixed state. The eigenvalues α_ℓ represent the probability for the system to be in the state ϕ_ℓ.

Any observable defined by a Hermitian operator A on X gives rise to an observation $\langle A \rangle_\rho$ on the system modeled by ρ according to the formula

$$\langle A \rangle_\rho = \mathrm{Tr}\{\rho A\},$$

where ρA denotes the operator multiplication of ρ and A. Examples of such observables are the mean position defined by the position operator X which operates through the multiplication by x, or the mean momentum defined by the momentum operator $P = -i\hbar\nabla_x$ where $\hbar$ is the reduced Planck constant and $i^2 = -1$. More generally, we shall consider operators $\mathrm{Op}(a)$ obtained from any symbol $a(x, p)$ of the position x and momentum p through the Weyl quantization by

$$\mathrm{Op}(a)\,\phi = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^{2d}} a\left(\frac{x+y}{2}, p\right) \phi(y)\, e^{i\frac{p(x-y)}{\hbar}}\, dp\, dy. \tag{3.2}$$

The Weyl quantization is such that any real valued symbol gives rise to a Hermitian operator (under regularity conditions that we shall not detail see for instance ref. 34). The Weyl quantization (3.2) is formally related to the Wigner transform (1.3) via the formula $\rho = (2\pi\hbar)^d \operatorname{Op}(f_w)$. Thus, Weyl quantization and Wigner transform are (up to a factor $(2\pi\hbar)^d$) inverse operations one to each other and

$$\operatorname{Tr}(\rho \operatorname{Op}(a)) = \int_{\mathbb{R}^{2d}} a(x, p)\, f_w(x, p)\, dx\, dp \tag{3.3}$$

holds. Wigner functions are therefore a convenient tool to express local moments in quantum mechanics. Entropy principles, however, are better expressed in terms of density matrices and operators. A class of symbol that we shall be particularly interested in are $a(x, p) = \lambda(x) \cdot \kappa(p)$ where $\lambda = (\lambda_i(x))_{i=0,\ldots,N}$ is an arbitrary $N+1$-tuple of real valued functions and $\kappa = (\kappa_i(p))_{i=0,\ldots,N}$ is the $N+1$-tuple of moment monomials.

We now choose a given $N+1$-tuple of real valued moment monomials κ, such that $\kappa_0(p) = 1$. For any given operator ρ, we shall denote by $K_\lambda(\rho)$ the expectation value of the operator $\operatorname{Op}(\lambda(x) \cdot \kappa(p))$ (denoted $\operatorname{Op}(\lambda \cdot \kappa)$ for short), i.e., for any $N+1$-tuple of real valued functions $\lambda = (\lambda_i(x))_{i=0,\ldots,N}$:

$$K_\lambda(\rho) = \operatorname{Tr}\{\rho \operatorname{Op}(\lambda \cdot \kappa)\} = \int_{\mathbb{R}^{2d}} \lambda(x) \cdot \kappa(p)\, f_w(x, p)\, dx\, dp. \tag{3.4}$$

$K_\lambda(\rho)$ is therefore the observation corresponding to a certain combination of the moment monomials $\kappa_i(p)$, weighted by x-dependent factors $\lambda_i(x)$. The mapping $\lambda \to K_\lambda(\rho)$ is a linear functional defined on the set of real valued functions $\lambda(x)$ which, by duality, defines a $N+1$-tuple of real valued functions $m[\rho] := m(x) = (m_i(x))_{i=0,\ldots,N}$, which are *functions of* x, according to

$$K_\lambda(\rho) = \int_{\mathbb{R}^d} \lambda(x) \cdot m(x)\, dx, \qquad \forall \lambda(x) \text{ real valued.} \tag{3.5}$$

These moments are nothing but the local moments of the Wigner distribution function f_w in the usual sense:

$$m[\rho](x) = \int \kappa(p)\, f_w(x, p, t)\, ds\, dp.$$

Therefore, (3.5) is a way to express local moments of the Wigner distribution function in terms of the density operator ρ. This formula is clearly the

quantum equivalent of (2.7). Therefore, in the quantum framework, there is no local relation between ρ and its moments m, but rather, a functional one, through the duality (3.5).

For the sake of clarity, we give explicit expressions of the moments $m[\rho]$ expressed in terms of the density matrix ρ. The proof of the following two lemmas is just an exercise in Fourier transforms using the definition (1.3) of the Wigner function f_w and the equivalence formula (3.3), and is left to the reader. We start with the following expression of $\mathrm{Op}(\lambda \cdot \kappa)$.

Lemma 3.1. Let $\beta = (\beta_1, \ldots, \beta_d) \in \mathbb{N}^d$ be a multi-index (with $\mathbb{N}$ the set of natural integers) and denote by $p^\beta = p_1^{\beta_1} \cdots p_d^{\beta_d}$ and $\partial/\partial x^\beta = \partial/\partial x_1^{\beta_1} \cdots \partial/\partial x_d^{\beta_d}$. Then, for any smooth real or complex-valued function $v(x)$, we have the two following equivalent expressions of the operator $\mathrm{Op}(p^\beta v)$:

$$\mathrm{Op}(p^\beta v)\,\phi = (-i\hbar)^{|\beta|} \sum_{\gamma_1=0}^{\beta_1} \cdots \sum_{\gamma_d=0}^{\beta_d} \binom{\beta_1}{\gamma_1} \cdots \binom{\beta_d}{\gamma_d} \frac{1}{2^{|\gamma|}} \frac{\partial v}{\partial x^\gamma} \frac{\partial \phi}{\partial x^{\beta-\gamma}}, \tag{3.6}$$

$$\mathrm{Op}(p^\beta v) = \frac{1}{2^{|\beta|}} \sum_{\gamma_1=0}^{\beta_1} \cdots \sum_{\gamma_d=0}^{\beta_d} \binom{\beta_1}{\gamma_1} \cdots \binom{\beta_d}{\gamma_d} p^\gamma v p^{\beta-\gamma}, \tag{3.7}$$

where $|\beta| = \beta_1 + \cdots + \beta_d$ and $\binom{\beta_i}{\gamma_i}$ is the binomial coefficient. We denote by v the multiplication operator by the function $v(x)$. Because v does not commute with p_i, the orders of the factors in the right-hand side of (3.7) matters.

The local moments are given as operators acting on the integral kernel of the operator ρ by:

Lemma 3.2. Let $\beta \in \mathbb{N}^d$ be a multi-index and let $m_\beta[\rho]$ be the moment of ρ associated with the monomial p^β, i.e., satisfying

$$m_\beta(x) = \int_{\mathbb{R}^d} p^\beta f_w(x, p)\, dp, \qquad \mathrm{Tr}\{\rho\, \mathrm{Op}(p^\beta v(x))\} = \int_{\mathbb{R}^d} m_\beta(x)\, v(x)\, dx,$$

for any test function $v(x)$. Let $\rho(x, x')$ be the integral kernel of the operator ρ in the position representation, i.e., the operator ρ acts on any square integrable function $\phi(x)$, $x \in \mathbb{R}^d$ according to

$$\rho\phi(x) = \int_{\mathbb{R}^d} \rho(x, x')\, \phi(x')\, dx'. \tag{3.8}$$

Then, m_β is given by

$$m_\beta(x) = \left(\frac{i\hbar}{2}\right)^{|\beta|} \sum_{\gamma_1=0}^{\beta_1} \cdots \sum_{\gamma_d=0}^{\beta_d} \binom{\beta_1}{\gamma_1} \cdots \binom{\beta_d}{\gamma_d} (-1)^{|\gamma|} \left(\frac{\partial}{\partial x^\gamma} \frac{\partial}{\partial x'^{(\beta-\gamma)}} \rho \right)\Big|_{(x,\,x)}. \tag{3.9}$$

This lemma shows that, as soon as the integral kernel $\rho(x, x')$ is smooth enough, the moment m_β is a function. Otherwise, m_β may be a singular distribution.

Now, we turn to the definition of entropy. By functional calculus, any continuous function h (and by duality, any measure) defined on the interval $\mathbb{R}_+$ gives rise to an operator $h(\rho)$ defined by

$$h(\rho)\,\phi = \sum_{\ell=1}^{\infty} h(\alpha_\ell)(\phi, \phi_\ell)_X\, \phi_\ell,$$

where $(\cdot, \cdot)_X$ denotes the scalar product in X (supposed linear with respect to the left entry and antilinear with respect to the right entry). Let h be a strictly convex function on $\mathbb{R}_+$. Then, we define the quantum entropy H of ρ with respect to h according to

$$H(\rho) = \mathrm{Tr}\{h(\rho)\}. \tag{3.10}$$

We now formulate the quantum entropy minimization principle: let $m(x)$ be a $N+1$-tuple of moment functions (defined on $\mathbb{R}^d$) such that $\int m_0\, dx = 1$. Find ρ^m such that

$$H(\rho^m) = \min \left\{ H(\rho) \mid \rho \text{ satisfies } K_\lambda(\rho) = \int_{\mathbb{R}^d} \lambda(x) \cdot m(x)\, dx, \right.$$
$$\left. \forall \text{ real valued } \lambda(x) = (\lambda_i(x))_{i=0,\ldots,N} \right\}. \tag{3.11}$$

We see that this minimization problem is the quantum equivalent of problem (2.6). The constrained optimization problem (3.11) can be rephrased as a saddle-point problem for the Lagrangian

$$\mathscr{L}_m(\rho, \lambda) = H(\rho) - \left(K_\lambda(\rho) - \int_{\mathbb{R}^d} m(x) \cdot \lambda(x)\, dx \right), \tag{3.12}$$

according to

$$H(\rho^m) = \min_\rho \max_\lambda \mathscr{L}_m(\rho, \lambda) = \max_\lambda \min_\rho \mathscr{L}_m(\rho, \lambda), \tag{3.13}$$

where now the minimum over ρ or the maximum over λ are unconstrained problems. Again, we stress the fact that $\lambda = (\lambda_i(x))_{i=0,\ldots,N}$ is a $N+1$-tuple of *functions of* x.

To pursue the analysis, we need the following two lemmas, the proofs of which are deferred to Appendix B. From now on, derivatives denoted with a δ will refer to Gâteaux derivatives. The Gâteaux derivative $\delta H/\delta\rho$ of a function $H(\rho)$ (if it exists) is a linear form acting on increments $\delta\rho$ according to

$$\frac{\delta H}{\delta \rho}\,\delta\rho = \lim_{t\to 0}\left\{\frac{1}{t}\left[H(\rho + t\,\delta\rho) - H(\rho)\right]\right\}.$$

A necessary condition for extremality of H is that its Gâteaux derivative vanishes (first order Euler–Lagrange equation of the extremality problem).

Lemma 3.3. Let h be a strictly increasing continuously differentiable function defined on $\mathbb{R}_+$. Consider that $H(\rho)$ is defined on the space of Trace-class positive self-adjoint operators ρ. Then H is Gâteaux differentiable and its Gâteaux derivative $\delta H/\delta\rho$ is given by:

$$\frac{\delta H}{\delta \rho}\,\delta\rho = \sum_{\ell=1}^{\infty} h'(\alpha_\ell)\,\delta\rho_{\ell\ell} = \mathrm{Tr}\{h'(\rho)\,\delta\rho\}, \tag{3.14}$$

where α_ℓ are the eigenvalues of ρ, and $\delta\rho_{\ell\ell}$ are the diagonal values of the perturbation operator $\delta\rho$ in the basis of the eigenfunctions ϕ_ℓ of ρ.

Lemma 3.4. Let h be a strictly convex twice continously differentiable function on $\mathbb{R}_+$. Then, H is strictly convex and is twice Gâteaux-differentiable, with:

$$\frac{\delta^2 H}{\delta \rho^2}(\delta\rho, \delta\rho) = \sum_{\ell, r} \frac{h'(\alpha_\ell) - h'(\alpha_r)}{\alpha_\ell - \alpha_r}\,|\delta\rho_{\ell r}|^2, \tag{3.15}$$

where the quotient is understood to be $h''(\alpha_\ell)$ when $\alpha_\ell = \alpha_r$. The perturbation operator $\delta\rho$ is assumed Hermitian.

In fact, Nier[30] has proved infinite Frechet differentiability of h (provided h is a C^∞ function) and has given proofs of formulae (3.14) and (3.15). However, his proof uses the theory of Hellfer and Sjöstrand[21] of almost analytic extensions in functional calculus. In the appendix, for the reader's convenience, we give elementary proofs of the weaker statements (3.14) and (3.15).

Let us now consider the unconstrained problem

$$\mathscr{L}_m(\rho_\lambda, \lambda) = \min_\rho \mathscr{L}_m(\rho, \lambda). \tag{3.16}$$

Then, we have:

Lemma 3.5. The necessary condition for extremality for the unconstrained minimization problem (3.16) is

$$\rho_\lambda = (h')^{-1}(\mathrm{Op}(\lambda \cdot \kappa)) \tag{3.17}$$

where $(h')^{-1}$ is the inverse function of h'.

The operator ρ_λ is called the equilibrium density operator associated with the $N+1$-tuple λ of entropic variables. We stress the fact that, in this theory, λ is a $N+1$-tuple of functions of the position variable x and not mere constants. Formula (3.17) must be understood in the sense of functional calculus, which is possible via the spectral theorem, since the operator $\mathrm{Op}(\lambda \cdot \kappa)$ is Hermitian.[31] The proof of Lemma 3.5 is deferred to Appendix A.

Now, the solution ρ^m of the constrained minimization problem (3.11) is an equilibrium density operator ρ_λ where $\lambda = \mu^m$ is a solution of the unconstrained maximization problem

$$H(\rho^m) = \mathscr{L}_m(\rho_{\mu^m}, \mu^m) = \max_\lambda \mathscr{L}_m(\rho_\lambda, \lambda). \tag{3.18}$$

We have:

Lemma 3.6. The solution ρ^m of the constrained Gibbs minimization problem (3.11) or equivalently, of the unconstrained maximization problem (3.18) is given by

$$\rho^m = \rho_{\mu^m}, \tag{3.19}$$

where μ^m is such that

$$K_\lambda(\rho_{\mu^m}) = \int_{\mathbb{R}^d} m(x) \cdot \lambda(x)\, dx, \qquad \forall \lambda(x). \tag{3.20}$$

By duality, relation (3.20) expresses that the moments of ρ_{μ^m} are m (see (3.5)). It is the quantum extension of (2.15). Again, the entropic variables μ

(which are functions of x) and the moment (or conservative) variables m (which are also functions of x) are dual (in the Legendre transform sense) through the fluid entropy (which is now a functional on functions of x, see Section 4). For the proof see Appendix A.

4. THE QUANTUM FLUID ENTROPY

We now discuss the concept of fluid entropy in the framework of the present theory. Let $m = (m_i(x))_{i=0,\ldots,N}$ be a given N-tuple of fluid moments (which are functions of the position variable x). We define the fluid entropy $\mathcal{S}(m)$ by

$$\mathcal{S}(m) = H(\rho^m). \tag{4.1}$$

For $\mathcal{S}$, we can prove:

Lemma 4.1.

(i) $\mathcal{S}$ is strictly convex.

(ii) We have

$$\frac{\delta \mathcal{S}}{\delta m} = \mu^m, \tag{4.2}$$

where $\delta \mathcal{S}/\delta m$ is the Gâteaux derivative of $\mathcal{S}$ with respect to m.

Equation (4.2) shows another aspect of the duality between μ and m, namely that they are dual through the entropy. Of course, this relation extends a well-known relation in the classical case. The proof can be found in Appendix A.

To highlight the duality between the entropic variables μ and the moments (or conservative variables) m, we show how relation (4.2) can be inverted by means of the Legendre dual of the entropy. Define

$$\Sigma(\mu) = \mathcal{S}(m) - \int_{\mathbb{R}^d} \mu \cdot m \, dx, \tag{4.3}$$

where m is such that $(\delta \mathcal{S}/\delta m)(m) = \mu$ (or in other words, such that $\mu^m = \mu$, i.e., m is the set of moment of ρ_μ). We have the following lemma, the proof of which is given in Appendix A.

Lemma 4.2.

(i) Σ is strictly concave.

(ii) We have

$$\frac{\delta \Sigma}{\delta \mu} = -m. \tag{4.4}$$

The function Σ is sometimes called the Massieu–Planck function.[4]

Remark 4.1. In equilibrium statistical mechanics (see, e.g., ref. 4) the constraints are global, i.e., are written

$$\mathrm{Tr}\{\rho \kappa_i\} = m_i, \qquad \forall i = 0,\ldots, N,$$

where $(\kappa_i)_{i=0,\ldots,N}$ are the operators corresponding to the global observables (e.g., the total energy: $\kappa = \hat{H}$) and $(m_i)_{i=0,\ldots,N}$ are $N+1$ real numbers. Among these constraints, the first one, corresponding to $\kappa_0 = 1$ and $m_0 = 1$, has a special status. Indeed, it does not say anything about the thermodynamical state of the system, but simply expresses that ρ is a statistical operator, i.e., satisfies (3.1). The associated equilibrium is written:

$$\rho_\mu = (h')^{-1}\left(\mu_0 + \sum_{i=1}^{N} \mu_i \kappa_i\right),$$

where μ_i are now constants. If we further specialize to the Boltzmann entropy (2.22), we get:

$$\rho_\mu = \exp\left\{\frac{1}{k_B}\left(\mu_0 + \sum_{i=1}^{N} \mu_i \kappa_i\right)\right\} = \frac{1}{Z}\exp\left\{\frac{1}{k_B}\left(\sum_{i=1}^{N} \mu_i \kappa_i\right)\right\}, \tag{4.5}$$

where Z is the so-called partition function. Z can be viewed as a function of $\mu_1,\ldots, \mu_N$ if ρ_μ is constrained to satisfy (3.1), indeed:

$$Z\{\mu_1,\ldots, \mu_N\} = \mathrm{Tr}\left\{\exp\left\{\frac{1}{k_B}\left(\sum_{i=1}^{N} \mu_i \kappa_i\right)\right\}\right\}.$$

It can be shown that $\ln Z$ coincides with $-\Sigma$ (up to a constant), i.e., we have:

$$\frac{\delta \ln Z}{\delta \mu_i} = m_i, \qquad i = 1,\ldots, N.$$

In our case however, since the μ_i's are no longer constant but instead functions of x, it is impossible to factor out the contribution of μ_0 outside the exponential. This is because $\mu_0(x)$ and $\sum_i \mu_i(x)\,\kappa_i$ are operators which do not commute in general. So, in our framework, there is no such object as a partition function. However, the Massieu function Σ is well-defined by (4.3) and can be used to define the moments m as functionals of the Lagrange multipliers μ. ▮

Remark 4.2. At this point, it is appropriate to compare our approach to the NESOM theory (for Non-Equilibrium Statistical Operator Mechanics), which has been pioneered by Zubarev *et al.* (see, e.g., ref. 36) and has been later expanded by Luzzi, Vasconcellos, and coworkers. The reader can refer, e.g., to refs. 27 and 28 for reviews. This approach consists in extending formula (4.5) into a formula for a *local equilibrium* according to

$$\rho_\mu = \frac{1}{Z}\exp\left\{\frac{1}{k_B}\left(\sum_{i=1}^{N}\int \mu_i(r,t)\,\kappa_i(r,t)\,dr\right)\right\}, \tag{4.6}$$

where $\kappa_i(r,t)$ are local versions of the moment operators κ corresponding to the conserved quantities.

The expression $\int \mu_i(r,t)\,\kappa_i(r,t)\,dr$ inside the exponential bears strong similarities with our introduction of the observable $\mu\cdot\kappa$ and formula (4.6) is close to our formula (3.17) which, in the case of the Boltzmann entropy (2.22), would reduce to

$$\rho_\mu = \exp\left\{\frac{1}{k_B}(\mathrm{Op}(\mu\cdot\kappa))\right\}. \tag{4.7}$$

In the cited references, the local operators $\kappa_i(r,t)$ are not further precised. If we assume that they are localizations of the global moment operators $\kappa_i(p)$ in the way outlined in the introduction, i.e., something like $\kappa_i(r,t) = \mathrm{Op}(\kappa_i(p)\,\delta(x-r))$, then the expression $\sum_i \int \mu_i(r,t)\,\kappa_i(r,t)\,dr$ coincides with $\mathrm{Op}(\mu\cdot\kappa)$. However, unless this is identification is made, the two approaches do not give the same results. Also, as pointed out in the previous remark, the factoring out of partition function in (4.6) looks somehow suspicious. However, the two approaches have clearly similar roots and the added value of our approach is to provide a neat mathematical framework to the notion of locally conserved variables by means of the operators $\mathrm{Op}(\mu\cdot\kappa)$ and the dual concept of moments, as developed in Section 3. This framework may in turn prove powerful for future extensions and applications of the theory. ▮

5. QUANTUM MOMENT HYDRODYNAMICS

5.1. General Framework

The time evolution of the density matrix can de derived from the Schrödinger equation and is given by the quantum Liouville equation for the density matrix (or von Neumann equation):

$$i\hbar \frac{\partial \rho}{\partial t} = [\hat{H}, \rho] + i\hbar Q(\rho), \tag{5.1}$$

where $\hat{H}$ is the particle Hamiltonian, $[\hat{H}, \rho] = \hat{H}\rho - \rho\hat{H}$ is the commutator of $\hat{H}$ and ρ and $Q(\rho)$ is an abstractly defined collision operator taking care of dissipation phenomena. To fix the ideas, we can think of $\hat{H}$ as being the simple Hamiltonian on $\mathbb{R}^d$

$$\hat{H}\phi = -\frac{\hbar^2}{2m^*}\Delta\phi + V\phi = \mathrm{Op}\left(\frac{|p|^2}{2m^*} + V\right)\phi, \tag{5.2}$$

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

About the collision operator Q, we specifically request the following:

(i) Q locally conserves the moments associated with $\kappa(p)$, i.e.,

$$\int Q_w(f_w)(x, p)\, \kappa_i(p)\, dp = 0, \qquad i = 0, \ldots, N, \quad \forall x \in \mathbb{R}^3,$$

where Q_w is the Wigner transform of Q.

(ii) $Q(\rho)$ dissipates the quantum entropy, i.e.,

$$\mathrm{Tr}\{Q(\rho)\, h'(\rho)\} \leqslant 0.$$

An example of such an operator is the BGK operator of Section 5.5 (we shall prove in ref. 8 that it is consistent with entropy dissipation, i.e., that property (ii) holds). In ref. 10, we also derive a Boltzmann-like collision operator for binary quantum collisions precisely on the basis of these two requirements.

From (5.1), we want to derive a system of conservation equations using a similar route as that exposed in Section 2 for the classical case. First, from (5.1) we derive a system of equations for the moments, and then, use the equilibrium density matrix ρ_λ to express all the quantities that cannot be directly expressed as moments. However, there is a significant difference from the classical case, in that the moments are not defined

directly but rather, from duality through the linear forms $K_\lambda(\rho)$. Therefore, the moment equations come naturally in duality form (or in weak form, in the sense of Partial Differential Equations theory).

Define $m[\rho]$ to be the moments of ρ, through the duality relation (3.5). To obtain the moment equations, we compose (5.1) on the right by $\mathrm{Op}(\lambda \cdot \kappa)$ and take the trace. We obtain:

$$\frac{\partial}{\partial t} \int_{\mathbb{R}^d} m[\rho(t)](x) \cdot \lambda(x)\, dx = \mathrm{Tr}\left\{ \left(\left[-\frac{i}{\hbar} \hat{H}, \rho \right] + Q(\rho) \right) \mathrm{Op}(\lambda \cdot \kappa) \right\}, \quad \forall \lambda(x). \tag{5.3}$$

Equation (5.3) is the quantum equivalent of (2.3). However, the right-hand side cannot be expressed in general in terms of the moments $m[\rho(t)]$. This is the closure problem.

We close Eq. (5.3) by using the solution $\rho^m = \rho_{\mu^m}$ of the Gibbs minimization problem (3.11) with moments $m = m[\rho(t)]$. We find

$$\frac{\partial}{\partial t} \int_{\mathbb{R}^d} m(x, t) \cdot \lambda(x)\, dx = \mathrm{Tr}\left\{ \left(\left[-\frac{i}{\hbar} \hat{H}, \rho_{\mu^{m(t)}} \right] + Q(\rho_{\mu^{m(t)}}) \right) \mathrm{Op}(\lambda \cdot \kappa) \right\}, \qquad \forall \lambda(x). \tag{5.4}$$

Equation (5.4) is a quantum moment closure system for the set of moments m, which we refer to as "Quantum Moment Hydrodynamics." Rewriting (5.4) in terms of Wigner functions instead of density matrices, one can now return to a strong formulation of the moment system. Equation (5.4) is equivalent to the weak formulation of

$$\partial_t m + \int_{\mathbb{R}^d} \kappa(p) \left\{ \nabla_x \cdot \left(\frac{1}{m^*} p f_w^m \right) - \theta[V]\, f_w^m \right\} dp = \int_{\mathbb{R}^d} \kappa(p)\, Q_w(f_w^m)\, dp, \tag{5.5}$$

where $f_w^m(x, p, t)$ is the closure Wigner function corresponding to $\rho_{\mu^{m(t)}}$, i.e.,

$$f_w^m(x, p, t) = (2\pi\hbar)^{-d}\, \mathrm{Op}^{-1}(\rho_{\mu^{m(t)}}) = (2\pi)^{-d} \int_{\mathbb{R}^d} \rho_{\mu^{m(t)}} \left(x - \frac{\hbar}{2} \eta, x + \frac{\hbar}{2} \eta \right) e^{i\eta \cdot p}\, d\eta \tag{5.6}$$

holds.

We now investigate several examples and consequences of this methodolgy. In all these examples, otherwise explicitely stated, we shall restrict to the case of the Hamiltonian (5.2).

5.2. Quantum Hydrodynamics

Our first use of the present framework is the derivation of the quantum hydrodynamic equations, which are the quantum counterpart of the classical hydrodynamic system (2.25)–(2.27). For this purpose, we again consider the $d+2$-tuple of moment functions (2.21), i.e., $\kappa(p) = (1, (p_i)_{i=1,\dots,d}, |p|^2/(2m^*))$. We first derive the moment equations from the Wigner function formulation (5.5). In analogy to the classical case, change from the moment variables m_i to density n, ensemble velocity u and temperature T via the formulas

$$m_0 = n = \int_{\mathbb{R}^d} f_w^m \, dp, \qquad m_i = q_i = m^* n u_i = \int_{\mathbb{R}^d} p_i f_w^m \, dp, \qquad i = 1,\dots, d$$

$$m_{d+1} = W = \frac{n(m^* |u|^2 + dk_B T)}{2} = \int_{\mathbb{R}^d} \frac{|p|^2}{2m^*} f_w^m \, dp.$$

The moment system (5.5) is then of the form

$$\begin{aligned}
&\text{(a)} \quad \partial_t n + \nabla_x \cdot (nu) = 0, \\
&\text{(b)} \quad \partial_t m^* nu + \nabla_x \cdot (m^* uu^T n + P) + n \nabla_x V = \langle p \rangle_{\text{coll}}, \\
&\text{(c)} \quad \partial_t n(m^* |u|^2 + dk_B T) + \nabla_x \cdot [n(m^* |u|^2 + dk_B T) u + 2Pu + 2q_H] \\
&\qquad + 2n \nabla_x V \cdot u = \left\langle \frac{|p|^2}{m^*} \right\rangle_{\text{coll}}
\end{aligned} \tag{5.7}$$

with the pressure tensor P and the heat flux q_H given by

$$\begin{aligned}
P &= \frac{1}{m^*} \int_{\mathbb{R}^d} (p - m^* u)(p - m^* u)^T f_w^m \, dp, \\
2q_H &= \frac{1}{(m^*)^2} \int_{\mathbb{R}^d} |p - m^* u|^2 (p - m^* u) f_w^m \, dp.
\end{aligned} \tag{5.8}$$

The closure, i.e., P and q_H, has to be computed using the closure Wigner function f_w^m which in turn is given by the closure operator ρ_{μ^m} via (5.6). Note that the quantum hydrodynamic equations coincide with the classical hydrodynamic system (2.25)–(2.27), except for the form of the pressure tensor P and the heat flux q_H. (For the Maxwellian closure (2.23), $P = k_B nTI$ and $q_H = 0$ holds.) The terms $\langle p \rangle_{\text{coll}}$ and $\langle \frac{|p|^2}{m^*} \rangle_{\text{coll}}$ on the right hand side of (5.7) denote the corresponding moments of the collision operator evaluated at f_w^m and have to be computed from the closure in

terms of n, u, T in the same way as the pressure tensor and the heat flux. They vanish identically in the case when collision operator Q_w conserves mass momentum and energy.

We now turn to the computation of f_w^m and ρ_{μ^m}. Let λ be a Lagrange multiplier, i.e., a $d+2$-tuple of real valued functions of x. Using the interpretation of classical thermodynamics, we can write $\lambda = (\frac{\mu_c}{\bar{T}}, \frac{\bar{u}}{\bar{T}}, -\frac{1}{\bar{T}})$ where $\mu_c(x)$, $\bar{u}(x)$, and $\bar{T}(x)$ will be called respectively local chemical potential, velocity and temperature. Note that $\bar{u}$ and $\bar{T}$ will in general be different from the ensemble velocity and temperature u and T in (5.7) which are defined directly from the moments of the Wigner function, in contrast with the classical case for which $u = \bar{u}$ and $T = \bar{T}$ holds. Then:

$$\lambda(x) \cdot \kappa(p) = \frac{1}{\bar{T}(x)} \left(\mu_c(x) + \bar{u}(x) \cdot p - \frac{|p|^2}{2m^*} \right). \tag{5.9}$$

A straightforward computation leads to the expression of $\mathrm{Op}(\lambda \cdot \kappa)$:

$$\begin{aligned} \mathrm{Op}(\lambda \cdot \kappa)\, \phi &:= \mathrm{Op}[\mu_c, \bar{u}, \bar{T}]\, \phi \\ &= \frac{\hbar^2}{2m^*} \nabla \cdot \left(\frac{1}{\bar{T}} \nabla \phi \right) - i\hbar \frac{1}{2} \left(\nabla \cdot \left(\frac{\bar{u}}{\bar{T}} \phi \right) + \frac{\bar{u}}{\bar{T}} \cdot \nabla \phi \right) \\ &\quad + \left(\frac{\mu_c}{\bar{T}} + \frac{1}{4} \frac{\hbar^2}{2m^*} \Delta \frac{1}{\bar{T}} \right) \phi. \end{aligned} \tag{5.10}$$

It is readily checked that $\mathrm{Op}[\mu_c, \bar{u}, \bar{T}]$ is a Hermitian operator.

Now, as soon as $\bar{T}(x) \geqslant 0$ a.e. (which we are going to assume from now on), $\mathrm{Op}[\mu_c, \bar{u}, \bar{T}]$ is an unbounded operator from below and is bounded from above. Thus, assuming that the spectrum of $\mathrm{Op}[\mu_c, \bar{u}, \bar{T}]$ consists of a discrete sequence of eigenvalues $(a_\ell[\mu_c, \bar{u}, \bar{T}])_{\ell = 1, \ldots, \infty}$, we have $\lim_{\ell \to \infty} a_\ell = -\infty$. Let us denote by ϕ_ℓ the associated Hilbert basis of eigenfunctions. By definition, the equilibrium operator $\rho_\lambda = \rho_{\mu_c, \bar{u}, \bar{T}} = (h')^{-1} \times (\mathrm{Op}[\mu_c, \bar{u}, \bar{T}])$ is given, for any $\phi \in X$ by:

$$\rho_{\mu_c, \bar{u}, \bar{T}} \phi = \sum_{\ell = 1}^{\infty} \alpha_\ell[\mu_c, \bar{u}, \bar{T}](\phi, \phi_\ell)_X\, \phi_\ell, \quad \alpha_\ell[\mu_c, \bar{u}, \bar{T}] = (h')^{-1} (a_\ell[\mu_c, \bar{u}, \bar{T}]). \tag{5.11}$$

Like in Section 2, let us denote by $m = (n, q, W)$ the vector of moments, with $n(x) > 0$ the probability of presence (satisfying $\int n(x)\, dx = 1$), $q(x) \in \mathbb{R}^d$ the mean momentum per particle, and $W(x)$ the mean energy per particle (i.e., respectively the density, momentum and energy divided by the total

number of particles $\mathcal{N}$). The equilibrium operator $\rho^{n,q,W}$, subject to the constraints (3.20) is a solution of the maximization problem (3.18), which, in the present case, is written:

$$\max_{\mu_c,\bar{u},\bar{T}} \left\{ \sum_{\ell=1}^{\infty} g(a_\ell[\mu_c,\bar{u},\bar{T}]) + \int_{\mathbb{R}^d} \left(\frac{\mu_c}{\bar{T}}(x)\, n(x) + \frac{\bar{u}}{\bar{T}}(x)\cdot q(x) - \frac{1}{\bar{T}}(x)\, W(x) \right) dx \right\}, \tag{5.12}$$

with $g(s) = h \circ (h')^{-1}(s) - s\,(h')^{-1}(s)$. We note that the first term in the curly bracket of (5.12) is nothing but the Massieu–Planck potential (4.3) and that (5.12) itself is a reformulation of relation (4.4) as a minimization problem.

Now, if we specialize to the Boltzmann entropy (2.22), we have $(h')^{-1}(s) = e^s$, $g(s) = -e^s$, and so $\rho_{\mu_c,\bar{u},\bar{T}} = \exp\{\mathrm{Op}[\mu_c,\bar{u},\bar{T}]\}$ is given by (5.11) with

$$\alpha_\ell[\mu_c,\bar{u},\bar{T}] = e^{a_\ell[\mu_c,\bar{u},\bar{T}]}. \tag{5.13}$$

Since $\rho_{\mu_c,\bar{u},\bar{T}}$ is a statistical operator, it satisfies (3.1) and therefore, we must have

$$\sum_{\ell=1}^{\infty} e^{a_\ell[\mu_c,\bar{u},\bar{T}]} = 1. \tag{5.14}$$

In particular, this implies that all eigenvalues of $\mathrm{Op}[\mu_c,\bar{u},\bar{T}]$ must be strictly negative or in other words, that $-\mathrm{Op}[\mu_c,\bar{u},\bar{T}]$ must be an elliptic operator. Furthermore, the eigenvalues must tend sufficiently fast to $-\infty$ for the series (5.14) to be convergent and have a sum equal to 1. Therefore, we must restrict the set of trial functions of the maximization problem to functions which guarantee such a property to the operator. Now, the optimization problem (5.12) for the Boltzmann entropy (2.22) is written:

$$\max_{\mu_c,\bar{u},\bar{T}} \left\{ -\sum_{\ell=1}^{\infty} e^{a_\ell[\mu_c,\bar{u},\bar{T}]} + \int_{\mathbb{R}^d} \left(\frac{\mu_c}{\bar{T}}(x)\, n(x) + \frac{\bar{u}}{\bar{T}}(x)\cdot q(x) - \frac{1}{\bar{T}}(x)\, W(x) \right) dx \right\}. \tag{5.15}$$

We can guess that this problem has some chances to have a unique solution. For instance, if we focus on the extremal value with respect to $\bar{T}$ (with fixed $\bar{u}/\bar{T}$ and $\mu_c/\bar{T}$), we see that $a_\ell[\mu_c,\bar{u},\bar{T}]$ is an increasing function of $\bar{T}$. Therefore, the first term in (5.15) is a decreasing function of $\bar{T}$ while the second term is an increasing one. Furthermore, as $\bar{T}$ approaches 0,

$a_\ell[\mu_c, \bar{u}, \bar{T}] \to -\infty$, $\exp a_\ell \to 0$ and the first term tends to 0, while the second one tends to $-\infty$ (we suppose that $W > 0$). Conversely, if $\bar{T} \to \infty$, we have $a_\ell[\mu_c, \bar{u}, \bar{T}] \to 0$, $\exp a_\ell \to 1$ and the sum diverges, making the first term tend to $-\infty$, while the second one tends to 0. Therefore, the expression to be maximized in (5.15) tends to $-\infty$ at the boundaries of the domain of variation of $\bar{T}$. Of course, this argument is not rigorous, since $\bar{T}$ is a function and some care has to be taken in making sense to the fact that $\bar{T}$ tends to 0 or to ∞. Also, the influence of the other parameters $\bar{u}/\bar{T}$ and $\mu_c/\bar{T}$ has to be studied. A rigorous investigation of this problem is deferred to future work.

In classical mechanics, the system of hydrodynamics equations is hyperbolic, i.e., the matrix of the derivatives of the flux functions with respect to the state variables is diagonalizable with real eigenvalues. These eigenvalues are the speeds of propagation of the various types of waves. Asking whether system (5.7) is hyperbolic in this sense would be meaningless. Indeed, since the flux functions are not local functions of the state variables, it would be meaningless to compute the matrix of derivatives in this way. Hyperbolicity provides a well-posedness theory, at least locally in time.[33, 35] The well-posedness of quantum hydrodynamics systems is an open problem so far. The fact that an entropy is decreasing in time as the following proposition states, should be an important ingredient in such a theory.

Proposition 5.1. Let the collision operator Q_w in (1.1) dissipate the entropy, i.e., let

$$\mathrm{Tr}\{Q(\rho)\, h'(\rho)\} \leqslant 0, \qquad \forall \rho, \tag{5.16}$$

hold. Then, any solution (n, u, T) of system (5.7) satisfies the entropy dissipation relation:

$$\frac{\partial}{\partial t}\, \mathscr{S}(n, q, W) \leqslant 0. \tag{5.17}$$

Proof. To prove the entropy conservation relation, we go back to the notation $m = (n, q, W)$ and use $\mu^m = (\mu_c/T, u/T, -1/T)$ for the Lagrange multiplier of the constraint m. We write, thanks to (4.2):

$$\frac{d}{dt}\, \mathscr{S}(m) = \frac{\delta \mathscr{S}}{\delta m}\, \frac{\partial m}{\partial t} = \int_{\mathbb{R}^d} \mu^m\, \frac{\partial m}{\partial t}\, dx.$$

Now, using (5.4) and the cyclicity of the trace, we have

$$\frac{d}{dt}\mathcal{S}(m) = \mathrm{Tr}\left\{-\frac{i}{\hbar}\hat{H}[\rho_{\mu^{m(t)}}, \mathrm{Op}(\mu^m \cdot \kappa)] + h'(\rho_{\mu^{m(t)}})\, Q(\rho_{\mu^{m(t)}})\right\}.$$

But, by construction, the operators $\mathrm{Op}(\mu^m \cdot \kappa)$ and $\rho_{\mu^{m(t)}}$ commute. Therefore, the right-hand side is less than zero and the result follows. ∎

We note that entropy conservation is not restricted to the quantum hydrodynamic model (5.7) but is valid for all quantum moment closure systems (5.4). In clasical hydrodynamics, it is a well established fact that the entropy of smooth solutions is constant in time. However, classical hydrodynamic models have discontinuous solutions (shock waves) the entropy of which is strictly decreasing with time. It is very unlikely that quantum hydrodynamic models exhibit shock waves solutions. The meaning of the model for discontinuous solutions would even be very unclear. For instance, what sense should we give to the operator (5.10) if the coefficients are discontinous functions?

Another interesting question is how the closure (5.7) and (5.8) relates to the Bohmian single state closure analyzed in refs. 16 and 17. The single state closure corresponds to the case of zero temperature, when all particles become statistically completely independent, i.e., the Boltzmann or Fermi–Dirac distribution reduces to a δ-function. Since, when using the Boltzmann entropy, we close the moment system essentially by $\exp(\mathrm{Op}(\mu\kappa))$ the same limit can probably be carried out by letting $T \to 0$ in (5.7a, b) for finite $\hbar$. Carrying out this limit is however not by no means simple, since it involves computing the limiting solution of the minimization problem.

5.3. Quantum Moment Hydrodynamics

With this term, we refer to all quantum moment closure systems (5.4) constructed from a larger basis of monomials than that of hydrodynamics. Therefore, we consider a finite subset $\mathscr{B}$ of $\mathbb{N}^d$ (where $\mathbb{N}$ is the set of natural integers) and consider multi-indices $\beta = (\beta_1, \ldots, \beta_d) \in \mathscr{B}$. We suppose that $0 \in \mathscr{B}$, $e_i \in \mathscr{B}$ for all $i \in \{1, \ldots, d\}$ (where $e_i = (\beta_j)_{j=1,\ldots,d}$ with $\beta_j = \delta_{ij}$). Let b be the cardinal of $\mathscr{B}$ and consider the b-tuple of moment monomials $\kappa(p) = (p^\beta)_{\beta \in \mathscr{B}}$. Additionally, we suppose that the space generated by $\kappa(p)$ contains $|p|^2$. In this way, it contains the hydrodynamic monomials $(1, p_i, |p|^2)$ and the associated quantum closure system (5.4) will contain the quantum hydrodynamic system (5.7) as a subcase. The vector κ may contain homogeneous polynomials which are not monomials, like $|p|^4$. However, for notational simplicity, we shall restrict to $\kappa(p)$ constructed

from simple monomials p^β and leave this straightforward extension to the reader.

We can now reproduce the procedure developed in the previous section. We just summarize it now. First, let us denote by $\lambda(x) = (\lambda_\beta)_{\beta \in \mathscr{B}}$ a b-tuple of Lagrange multipliers. Then, the operator $\mathrm{Op}(\lambda \cdot \kappa)$ is given by:

$$\mathrm{Op}(\lambda \cdot \kappa) = \sum_{\beta \in \mathscr{B}} \mathrm{Op}(\lambda_\beta \cdot p^\beta), \tag{5.18}$$

where the expression of $\mathrm{Op}(\lambda_\beta \cdot p^\beta)$ is given in Lemma 3.1.

From the analysis conducted in Section 5.2 (at least with the Boltzmann entropy (2.22)), the maximization problem (3.18) has a non-empty set of solutions only if there is a non-empty set of λ such that the operator $-\mathrm{Op}(\lambda \cdot \kappa)$ is elliptic. In fact, we shall request that the set of such λ has a non-empty interior. This condition is analogous to condition (III) of Levermore's approach[26] and is likely to lead to identical constraints on the set of monomials to be considered. This point will be investigated in more detail in future work. This requirement leads to a restriction on the possible sets $\mathscr{B}$.

We now suppose that this requirement is fulfilled and that the operator $\mathrm{Op}(\lambda \cdot \kappa)$ has a sequence of negative eigenvalues $(a_\ell[\lambda])_{\ell = 1, \ldots, \infty}$ such that $a_\ell[\lambda] \to -\infty$ as $\ell \to \infty$ and that the associated eigenvectors ϕ_ℓ form a complete orthonormal basis. Let us now denote by $m(x) = (m_\beta)_{\beta \in \mathscr{B}}$ a given set of moments. The maximization problem (3.18) is now stated as follows (from now on, we shall restrict to the case of the Boltzmann entropy (2.22)):

$$\max_\lambda \left\{ -\sum_{\ell=1}^{\infty} e^{a_\ell[\lambda]} + \int_{\mathbb{R}^d} \sum_{\beta \in \mathscr{B}} \lambda_\beta(x)\, m_\beta(x)\, dx \right\}. \tag{5.19}$$

Let us denote by μ^m the value of λ which solves this maximization problem (assuming that the solution exists and is unique) and $\rho^m = \rho_{\mu^m}$, the associated operator

$$\rho_{\mu^m}\, \phi = \sum_{\ell=1}^{\infty} \alpha_\ell[\mu^m](\phi, \phi_\ell)_X\, \phi_\ell, \qquad \alpha_\ell[\mu^m] = e^{a_\ell[\mu^m]}. \tag{5.20}$$

We shall derive the quantum moment hydrodynamics system in a similar form as for the quantum hydrodynamics system. The derivation of a form like (5.7) shall be done in a future work. Let us consider the βth component λ_β of an arbitrary λ and denote by $b^\beta_{\ell r}[\lambda_\beta]$ the matrix element of the operator $\mathrm{Op}(\lambda_\beta\, p^\beta)$ in the eigenbasis ϕ_ℓ of ρ^m. As in Section 5.2, we

denote by $\hat{H}_{\ell r}$ the matrix element of the Hamiltonian in the same basis, and by $Q_{\ell r}(\rho)$ the matrix element of $Q(\rho)$. We have:

$$\mathrm{Tr}\{[\hat{H}, \rho^m]\ \mathrm{Op}(\lambda_\beta p^\beta)\} = \sum_{\ell, r} \hat{H}_{\ell r}(\alpha_r - \alpha_\ell)\, b^\beta_{r\ell}[\lambda_\beta]. \tag{5.21}$$

Finally, the system of quantum moment hydrodynamics equations can be written according to:

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^d} m_\beta(x, t)\, \lambda_\beta(x)\, dx = -\frac{i}{\hbar}\sum_{\ell, r} \hat{H}_{\ell r}(\alpha_r - \alpha_\ell)\, b^\beta_{r\ell}[\lambda_\beta] + \sum_{\ell, r} Q_{\ell r}(\rho)\, b^\beta_{r\ell}[\lambda_\beta], \tag{5.22}$$

$$\forall \lambda_\beta(x), \qquad \forall \beta \in \mathscr{B}. \tag{5.23}$$

This provides an evolution system for the quantities m_β, which is well adapted to a Galerkin discretization. For this system also, provided that Q is entropy dissipative, (i.e., property (5.16) is satisfied), the entropy dissipation inequality (5.17) applies and the entropy $\mathscr{S}(m)$ is decreasing in time.

We point out that the solution of the maximization problem (5.20) does not always exist in the classical case (see, in particular, refs. 24 and 25). It is yet an open problem, and formidably more difficult, to solve it in the quantum case.

5.4. A Galerkin Discretization

The main difficulty in solving the quantum hydrodynamic model (5.7) is of course the evaluation of the pressure tensor and the heat flux vector through formulae (5.8). Indeed, this evaluation requires the solution of the optimization problem (5.12) or (5.15). We now roughly outline the computational complexity (and feasibility) of this problem. The moment equations (5.3) render themselves to a natural Galerkin discretization in space, which preserves the entropy principle. We start by choosing a set of scalar basis functions $\lambda_j(x)$, $j = 1,..., J$ in space and approximate the moment vector $m = (m_0,..., m_N)$ in (5.3) by

$$m_n(x, t) \approx \sum_{j=1}^{J} z^j_n(t)\, \lambda_j(x), \qquad n = 0,..., N. \tag{5.24}$$

Equation (5.3) is then replaced by

$$\int_{\mathbb{R}^d} \lambda_j(x)\, \partial_t m(x, t)\, dx = \mathrm{Tr}\left\{\left(-\frac{i}{\hbar}[\hat{H}, \rho^m] + Q(\rho^m)\right)\mathrm{Op}(\lambda_j \kappa)\right\}, \quad j = 1,..., J, \tag{5.25}$$

where ρ^m is the solution of the constrained minimization problem

$$\mathrm{Tr}(h(\rho^m)) = \min\left\{\mathrm{Tr}(h(\rho))\colon \mathrm{Tr}\{\rho\ \mathrm{Op}(\lambda_j\,\kappa)\} = \int_{\mathbb{R}^d} \lambda_j\, m\, dx,\ j = 1,\ldots,J\right\}. \tag{5.26}$$

Thus, we have replaced the minimization problem (3.11) by a problem with finitely many constraints leading, consequently to only $J(N+1)$ Lagrange multiplyers. Next, we replace the density matrix ρ in (5.26) by a finite expansion. We choose orthonormal basis functions $\psi_k(x)$, $k = 1,\ldots,K$, and approximate the density matrix ρ by

$$\rho^m(x, y) \approx \sum_{k,l=1}^{K} R^m_{kl} r_{kl}(x, y), \qquad r_{kl}(x, y) = \psi_k(x)\,\psi_l(y)^*,$$

where R^m_{kl} is a Hermitian matrix and the star exponent denotes complex conjugation. In order to arrive at a finite minimization problem, we also have to replace the operator $\mathrm{Op}(\lambda_j\kappa)$ by a finite matrix, i.e.,

$$\mathrm{Op}(\lambda_j\,\kappa) \approx \sum_{k,l=1}^{K} \Gamma^{jn}_{kl} r_{kl}(x, y),$$

$$\Gamma^{jn}_{kl} = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \psi_k(x)^*\,\mathrm{Op}(\lambda_j\kappa_n)(x, y)\,\psi_l(y)\,dx\,dy,$$

and replace the minimization problem (5.26) by

$$\mathrm{Tr}(h(R^m)) = \min\left\{\mathrm{Tr}(h(R))\colon \mathrm{Tr}\{R\Gamma^{jn}\} = \int_{\mathbb{R}^d} \lambda_j m_n\, dx,\ j = 1,\ldots,J,\ n = 0,\ldots,N\right\}. \tag{5.27}$$

The symbol Tr in (5.27) denotes now just the usual matrix trace and h is now to be understood as the function of a matrix. The Galerkin equations (5.25) are then replaced by

$$\int_{\mathbb{R}^d} \lambda_j(x)\,\partial_t m_n(x, t)\,dx$$

$$= \sum_{kl=1}^{K} \Gamma^{jn}_{kl}\,\mathrm{Tr}\left\{\left(-\frac{i}{h}[\hat{H}, \rho^m] + Q(\rho^m)\right) r_{kl}\right\}, \quad j = 1,\ldots,J, \quad n = 0,\ldots,N. \tag{5.28}$$

(5.28) is a system of ordinary differential equations for the expansion coefficients $z_n^j(t)$ after inserting (5.24) for the components m_n of the moment vector. The system (5.27)–(5.28) now clearly satisfies the same entropy relation as given by Proposition 5.1 on a discrete level. This can be seen by multiplying (5.28) by μ_{jn} and summation over j and n, where μ_{jn} is the Lagrange multiplier of the minimization problem (5.27), i.e., $h'(R^m) = \sum_{jn} \mu_{jn} \Gamma^{jn}$ holds. Two questions arise:

- How to choose the basis functions ψ_k for the density matrices and the basis functions λ_j for the moments?
- How large should K^2, the number of density matrix basis functions, be compared to J, the number of moment basis functions?

There is considerable freedom in the answer to the first question. One possibility would be to choose the ψ_k as the eigenfunctions of ρ^m itself, making the matrix R^m diagonal. This makes the evaluation of $h(R)$ trivial, but has the disadvantage that we have to compute the matrices Γ^{jn} and the matrix corresponding to the Hamiltonian $\hat{H}$ anew for each time step. It is probably preferable to choose a "good" basis $\{\psi_k\}$ (say eigenfunctions of the Hamiltonian, which are also the eigenfunctions of the equilibrium solution $e^{-\beta \hat{H}}$), compute the Γ^{jn} once and for all, and rather deal with the problem of computing the matrix function $h(R)$ in the optimization procedure. An alternative would be to use the entropy variables μ_{jn} as primary variables, since $R^m = (h')^{-1} (\sum_{jn} \mu_{jn} \Gamma^{jn})$ has to hold. This has the advantage of eliminating the optimization procedure but makes the ODE system (5.28) implicit, since the term on the left hand side of (5.28) is then given by

$$\int_{\mathbb{R}^d} \lambda_j m_n \, dx = \mathrm{Tr} \left\{ \Gamma^{jn} (h')^{-1} \left(\sum_{j'n'} \mu_{j'n'} \Gamma^{j'n'} \right) \right\}.$$

The easiest way to invert this equation might again be by using an optimization procedure (i.e., a discrete version of (5.19). As to the second question: The number of degrees of freedom in the minimization problem (5.27) is K^2 (the number of elements in a $K \times K$ hermitian matrix if we count real and imaginary parts separately). Therefore, $K^2 > J(N+1)$ has to hold, in order to have more variables than constraints. How much larger K^2 has to be will depend on how well we wish to approximate the minimization problem. This will have to be determined by numerical experiment.

We conclude this section with a remark about the usefulness of Wigner functions in this context. While Wigner functions are convenient for expressing local moments they are not the appropriate tool in this approach. The reason for this is the following. The reason why Wigner

functions were useful in expressing the moment equations is that the moments of $[H, \rho]$ can be expressed in terms of the moments of ρ in the Wigner picture, up to a few closure terms. This property is lost here, due to taking a finite number of expansion terms for the density matrix. If we define by f_{kl} the Wigner transform of the basis element ρ_{kl} of the density matrix, we obtain

$$\Gamma_{kl}^{jn} = \mathrm{Tr}\{\mathrm{Op}(\lambda_j \kappa_n)\, \rho_{kl}\} = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \lambda_j \kappa_n f_{kl}\, dr\, dp$$

and (5.28) becomes

$$\int_{\mathbb{R}^d} \lambda_j(x)\, \partial_t m_n(x, t)\, dx$$

$$= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \sum_{kl=1}^{K} \Gamma_{kl}^{jn} \left\{ -\nabla_x \left(\frac{1}{m^*} p f^m \right) + \theta[V]\, f^m + Q_w(f^m) \right\} f_{kl}\, dx\, dp,$$

$$j = 1, \ldots, J, \quad n = 0, \ldots, N. \tag{5.29}$$

Written out in more detail, the right hand side is of the form

$$\int_{\mathbb{R}^{4d}} \sum_{kl=1}^{K} \lambda_j(x')\, \kappa_n(p')\, f_{kl}(x', p')\, f_{kl}(x, p)$$

$$\times \left\{ -\nabla_x \left(\frac{1}{m^*} p f^m \right) + \theta[V]\, f^m + Q_w(f^m) \right\} (x, p)\, dx\, dp\, dx'\, dp'.$$

If now

$$\sum_{kl=1}^{K} f_{kl}(x', p')\, f_{kl}(x, p) = \delta(x' - x)\, \delta(p' - p)$$

were to hold, the right hand side of (5.29) would simplify in the same way as it did in Section 5.2. For a finite number K of expansion terms this can, however, not be assumed.

5.5. Quantum BGK Model

Finally, we end this section about the quantum moment hierarchies by outlining the use which can be made of the equilibrium density matrix ρ^m under the moment constraint m. Indeed, a density matrix equation including

relaxation to local equilibria can be written in the spirit of the BGK model of rarefied gas dynamics. Such a model can be written:

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[\hat{H}, \rho] - \nu_c(\rho - \rho^{m[\rho(t)]}), \tag{5.30}$$

where we haved denoted by $m[\rho(t)]$ the moments associated with ρ at time t according to (3.5). Usually, we shall take the hydrodynamic moments. We shall prove in ref. 8 that such an operator is consistent with entropy decay. The quantity ν_c is a collision frequency. By construction, composing on the right by $\mathrm{Op}(\lambda \cdot \kappa)$ where κ are the hydrodynamic monomials shows that the relaxation term $\rho - \rho^{m[\rho(t)]}$ does not appear in the evolution of the hydrodynamic moment equations (5.3). However, the scaling $\nu_c \to \nu_c/\varepsilon$, where $\varepsilon \ll 1$ is a small parameter representing the Knudsen number (i.e., the ratio of the collision scale to the macroscopic scale), allows to justify (at least formally) the hydrodynamic closure (5.4). In most of the literature, only relaxation towards global equilibria are taken into account through equilibria ρ^m associated with *global constraints* (like in Remark 4.1). The present approach allows to give a meaning to "local equilibrium relaxation" in a quantum framework. In fact, the term "local" is slightly misleading in this case. It refers to the fact that moment constraints are *functions of* x. However, the relation between the moment constraints m and the equilibrium density matrix ρ^m is not a local one, but a *functional* one.

A natural question is the existence of a series of perturbative models obtained through an expansion of the solutions of (5.30) in powers of ε (after rescaling $\nu_c \to \nu_c/\varepsilon$), in the spirit of the Chapman–Enskog expansion of the Boltzmann equation of gas dynamics (see ref. 26). This question will be investigated in future work.

Another question is related to the possible existence of "diffusion-like" limits of model (5.30) (after a simulatneous rescaling $\nu_c \to \nu_c/\varepsilon$ and $\partial\rho/\partial t \to \varepsilon\, \partial\rho/\partial t$, with $\varepsilon \ll 1$). This question is investigated in ref. 8.

6. CONCLUSION AND FUTURE WORK

We have developed a systematic approach to construct quantum hydrodynamical models from appropriate closures of the quantum Liouville equation. This approach is made possible by an adequate definition of the local moment of a density operator. This concept is defined by duality through the observations of the system on a suitable class of test functions. Then, the concept of an equilibrium density matrix, a solution of the entropy minimization principle subject to the constraints of given moments, is developed. Taking successive moments of the quantum Liouville equation

(in the above defined sense), it is possible to close the chain of equations by this equilibrium operator, giving rise to a hierarchy of models called Quantum Moment Hydrodynamic models. We have studied in more detail the quantum hydrodynamic model corresponding to the usual hydrodynamical moments and have shown that it is formally similar as the classical one apart from nonlocal expressions of the pressure tensor and heat-flux vector.

Obviously, this paper leaves a lot of mathematical questions open: existence of solutions for the entropy minimization problem, well-posedness of the quantum hydrodynamic equations, derivation of efficient numerical solvers, well-posedness of quantum BGK models, existence of perturbative series expansions of solutions in the spirit of the Chapman–Enskog expansion, derivation of quantum diffusion models (like the quantum drift-diffusion), etc. Other pending questions are concerned with the physical restriction of the model. One can think of taking into account nonconstant particle number (thus requesting the use of Fock spaces), Fermi–Dirac or Bose–Einstein statistics, spin and relativity effects together with the inclusion of the magnetic field through the Dirac equation, etc. All these questions clearly open a large field of investigations for the future.

APPENDIX A. QUANTUM ENTROPY MINIMIZATION PRINCIPLE: PROOFS

In this appendix, we give the proofs of the statements related with the quantum entropy minimization principle.

Proof of Lemma 3.5. The Euler–Lagrange equation for the minimization problem (3.16) is

$$\left(\frac{\delta \mathscr{L}_m}{\delta \rho}\right)\Big|_{(\rho_\lambda, \lambda)} = \left(\frac{\delta H}{\delta \rho}\right)\Big|_{\rho_\lambda} - \left(\frac{\delta K_\lambda}{\delta \rho}\right)\Big|_{\rho_\lambda} = 0. \tag{A.1}$$

Thanks to the linearity of $K_\lambda(\rho)$ with respect to ρ, we have, for any self-adjoint, trace class operator $\delta\rho$:

$$\left(\frac{\delta K_\lambda}{\delta \rho}\right)\Big|_{\rho} \delta\rho = \mathrm{Tr}\{(\delta\rho)\,\mathrm{Op}(\lambda\cdot\kappa)\} = \sum_{\ell, r} \delta\rho_{\ell r} a_{r\ell},$$

where we denote by $a_{\ell r}$ the matrix element of the operator $\mathrm{Op}(\lambda\cdot\kappa)$ in the eigenbasis of ρ. Then, thanks to (3.14), the Euler–Lagrange equation (A.1) is written:

$$\sum_{\ell=1}^{\infty} \left(h'(\alpha_\ell(\rho))\, \delta\rho_{\ell\ell} - \sum_{r=1}^{\infty} \delta\rho_{\ell r} a_{r\ell} \right) = 0,$$

for all Hermitian, trace class operators $\delta\rho$. Choosing $\delta\rho_{\ell' r'} = \delta_{\ell'\ell}\delta_{r' r} + \delta_{\ell' r}\delta_{r'\ell}$ or $\delta\rho_{\ell' r'} = i(\delta_{\ell'\ell}\delta_{r' r} - \delta_{\ell' r}\delta_{r'\ell})$ where $\delta_{\ell' r'}$ is the Kronecker symbol, with $\ell \neq r$, we deduce that $a_{\ell r}$ must be equal to zero, i.e., that ρ must be diagonal in the basis where the operator $\mathrm{Op}(\lambda \cdot \kappa)$ is diagonal. Such a basis always exist, since $\mathrm{Op}(\lambda \cdot \kappa)$ is Hermitian (because $\lambda(x)$ and $\kappa(p)$ are real functions) at least in the generalized sense, (i.e., in the sense of the spectral measure if $\mathrm{Op}(\lambda \cdot \kappa)$ has continuous spectrum, see ref. 31). Then, taking $\delta\rho_{\ell' r'} = \delta_{\ell' \ell}\delta_{r' \ell}$, we deduce that

$$h'(\alpha_\ell(\rho)) = a_{\ell\ell},$$

i.e.,

$$\alpha_\ell(\rho) = (h')^{-1}(a_{\ell\ell}),$$

which is precisely the definition of ρ being given by (3.17). ▮

Proof of Lemma 3.6. The Euler–Lagrange equation of the maximization problem reads (where we drop the superscript m):

$$\left(\frac{\delta \mathscr{L}_m}{\delta \rho}\right)\Big|_{(\rho_\mu, \mu)} \left(\frac{\delta \rho_\lambda}{\delta \lambda}\right)\Big|_\mu + \left(\frac{\delta \mathscr{L}_m}{\delta \lambda}\right)\Big|_{(\rho_\mu, \mu)} = 0. \tag{A.2}$$

But, by the Euler–Lagrange equation of the minimization problem (A.1), since ρ_μ realizes the minimum, the first term is identically zero. Therefore, μ is characterized by

$$\left(\frac{\delta \mathscr{L}_m}{\delta \lambda}\right)\Big|_\mu = 0.$$

By linearity of $\mathscr{L}_m$ with respect to λ, we have:

$$\left(\frac{\delta \mathscr{L}_m}{\delta \lambda}\right)\Big|_\mu \delta\lambda = -\left(\mathrm{Tr}\{\rho_\mu \mathrm{Op}(\delta\lambda \cdot \kappa)\} - \int_{\mathbb{R}^d} m(x) \cdot \delta\lambda(x)\, dx\right) = 0,$$

for any N-tuple $\delta\lambda = (\delta\lambda_i(x))_{i=1,\ldots,N}$ of arbitrary functions $\delta\lambda_i(x)$, which is exactly relation (3.20) (with $\delta\lambda = \lambda$). It is easy to show that this extremum is indeed a maximum. This classical point is left to the reader. ▮

Proof of Lemma 4.1.

(i) We use that H is strictly convex (by virtue of Lemma 3.4. Therefore, let m and m' be two moment vectors and $t \in [0, 1]$. Then:

$$\begin{aligned}
&\mathscr{S}(tm+(1-t)\,m') \\
&\quad = H(\rho^{tm+(1-t)\,m'}) \\
&\quad = \min\left\{ H(\rho) \mid \mathrm{Tr}\{\rho\ \mathrm{Op}(\lambda\cdot\kappa)\} = \int_{\mathbb{R}^d} \lambda\cdot(tm+(1-t)\,m')\,dx,\ \forall\lambda(x) \right\}.
\end{aligned}$$

But we have

$$\begin{aligned}
&\mathrm{Tr}\{(t\rho^m+(1-t)\,\rho^{m'})\ \mathrm{Op}(\lambda\cdot\kappa)\} \\
&\quad = t\ \mathrm{Tr}\{\rho^m\ \mathrm{Op}(\lambda\cdot\kappa)\}+(1-t)\ \mathrm{Tr}\{\rho^{m'}\ \mathrm{Op}(\lambda\cdot\kappa)\} \\
&\quad = t\int_{\mathbb{R}^d} \lambda\cdot m\,dx+(1-t)\int_{\mathbb{R}^d} \lambda\cdot m'\,dx \\
&\quad = \int_{\mathbb{R}^d} \lambda\cdot(tm+(1-t)\,m')\,dx.
\end{aligned}$$

Therefore, $t\rho^m+(1-t)\,\rho^{m'}$ satisfies the constraints and consequently:

$$H(\rho^{tm+(1-t)\,m'}) \leqslant H(t\rho^m+(1-t)\,\rho^{m'}).$$

Now, using the strict convexity of H, we have:

$$H(\rho^{tm+(1-t)\,m'}) < tH(\rho^m)+(1-t)\,H(\rho^{m'}),$$

or,

$$\mathscr{S}(tm+(1-t)\,m') < t\mathscr{S}(m)+(1-t)\,\mathscr{S}(m'),$$

which proves the strict convexity of $\mathscr{S}$, i.e., point (i).

(ii) We write:

$$\begin{aligned}
\frac{\delta\mathscr{S}}{\delta m} &= \frac{\delta}{\delta m}(\mathscr{L}_m(\rho_{\mu^m}, \mu^m)) \\
&= \frac{\delta\mathscr{L}_m}{\delta m}(\rho_{\mu^m}, \mu^m)+\left(\frac{\delta\mathscr{L}_m}{\delta\rho}(\rho_{\mu^m}, \mu^m)\,\frac{\delta\rho_\lambda}{\delta\lambda}(\mu^m)+\frac{\delta\mathscr{L}_m}{\delta\lambda}(\rho_{\mu^m}, \mu^m)\right)\frac{\delta\mu^m}{\delta m} \\
&= \frac{\delta\mathscr{L}_m}{\delta m}(\rho_{\mu^m}, \mu^m),
\end{aligned}$$

where the last equality follows from the fact that μ^m is a solution of the Euler–Lagrange equation (A.2). Therefore, for any perturbation $\delta m = (\delta m_i(x))_{i=1,\dots,N}$, we have

$$\frac{\delta \mathscr{S}}{\delta m}\,\delta m = \frac{\delta \mathscr{L}_m}{\delta m}\,(\rho_{\mu^m}, \mu^m)\,\delta m = \int_{\mathbb{R}^d} \mu^m(x)\cdot \delta m(x)\,dx,$$

which exactly means (4.2) by duality. ▮

Proof of Lemma 4.2.

(i) Σ can be defined as

$$\Sigma(\mu) = \min_m \left\{ \mathscr{S}(m) - \int_{\mathbb{R}^d} \mu\cdot m\,dx \right\},$$

and a minimum of linear functions, which are concave functions, is concave.

(ii) We have:

$$\frac{\delta \Sigma}{\delta \mu}\,\delta\mu = \frac{\delta \mathscr{S}}{\delta m}\frac{\delta m}{\delta \mu}\,\delta\mu - \int_{\mathbb{R}^d} \delta\mu\cdot m\,dx - \int_{\mathbb{R}^d} \mu\cdot\frac{\delta m}{\delta \mu}\,\delta\mu\,dx.$$

But, with (4.2), the first term of the right-hand side cancels the last one and we have

$$\frac{\delta \Sigma}{\delta \mu}\,\delta\mu = -\int_{\mathbb{R}^d} \delta\mu\cdot m\,dx,$$

which proves (4.4). ▮

APPENDIX B. PROPERTIES OF THE QUANTUM ENTROPY *H*

The proofs of Lemmas 3.3 and 3.4 can be found, e.g., in ref. 30. Here, we give an elementary proof of these results.

Proof of Lemmas 3.3 and 3.4. Let $\delta\rho$ be a self-adjoint trace-class operator. By the definition of the Gâteaux differentiability, we wish to investigate if the following limit exists:

$$\frac{\delta H}{\delta \rho}\,\delta\rho = \lim_{t\to 0}\left[\frac{1}{t}\left(\mathrm{Tr}\{h(\rho + t\delta\rho)\} - \mathrm{Tr}\{h(\rho)\}\right)\right].$$

We can choose variations $\delta\rho$ the expressions of which are given by either of the following formulae in the eigenbasis ϕ_ℓ of ρ:

$$\delta\rho_{\ell' r'} = \frac{\theta}{2}(\delta_{\ell'\ell}\delta_{r' r} + \delta_{\ell' r}\delta_{r'\ell}), \tag{B.1}$$

$$\delta\rho_{\ell' r'} = \frac{i\theta}{2}(\delta_{\ell'\ell}\delta_{r' r} - \delta_{\ell' r}\delta_{r'\ell}), \tag{B.2}$$

where $\delta_{\ell' r'}$ is the Kronecker symbol and θ is a real number. Indeed, any variation $\delta\rho$ can be decomposed into a (possibly infinite but convergent) sum of such variations. The elementary $\delta\rho$ is still trace-class and self adjoint. It is then enough to investigate the influence of the perturbation on the space spanned by (ϕ_ℓ, ϕ_r). We investigate the following three cases:

(i) $\ell = r$. Then, $\alpha_\ell(\rho + t\delta\rho) = \alpha_\ell(\rho) + t\theta$ and therefore,

$$h(\alpha_\ell(\rho + t\delta\rho)) = h(\alpha_\ell(\rho)) + t\theta\, h'(\alpha_\ell(\rho)) + \frac{t^2\theta^2}{2} h''(\alpha_\ell(\rho)) + o(t^2),$$

as $t \to 0$. Therefore, in this case,

$$\frac{\delta H}{\delta\rho}\delta\rho = h'(\alpha_\ell(\rho))\,\delta\rho_{\ell\ell}, \qquad \frac{\delta^2 H}{\delta\rho^2}(\delta\rho, \delta\rho) = h''(\alpha_\ell(\rho))\,|\delta\rho_{\ell\ell}|^2.$$

(ii) $\ell \neq r$ and $\alpha_\ell \neq \alpha_r$. Then, in the basis (ϕ_ℓ, ϕ_r), the matrix $\rho + t\delta\rho$ is written as follows (respectively in the cases (B.1) and (B.2)):

$$\rho + t\delta\rho = \begin{pmatrix} \alpha_\ell & \theta t/2 \\ \theta t/2 & \alpha_r \end{pmatrix} \quad \text{or} \quad \rho + t\delta\rho = \begin{pmatrix} \alpha_\ell & i\theta t/2 \\ -i\theta t/2 & \alpha_r \end{pmatrix}.$$

In these two cases, the eigenvalues of $\rho + t\,\delta\rho$ are the same. Suppose that $\alpha_\ell > \alpha_r$ to fix the ideas. Then, they are given by

$$\alpha_\ell(t) = \frac{1}{2}(\alpha_\ell + \alpha_r + \sqrt{(\alpha_\ell - \alpha_r)^2 + \theta^2 t^2}) = \alpha_\ell + \frac{t^2\theta^2}{4(\alpha_\ell - \alpha_r)} + o(t^2),$$

$$\alpha_r(t) = \frac{1}{2}(\alpha_\ell + \alpha_r - \sqrt{(\alpha_\ell - \alpha_r)^2 + \theta^2 t^2}) = \alpha_r - \frac{t^2\theta^2}{4(\alpha_\ell - \alpha_r)} + o(t^2),$$

as $t \to 0$. Thus,

$$h(\alpha_\ell(t)) + h(\alpha_r(t)) = h(\alpha_\ell) + h(\alpha_r) + \frac{t^2\theta^2}{4}\frac{h'(\alpha_\ell) - h'(\alpha_r)}{\alpha_\ell - \alpha_r} + o(t^2).$$

Therefore, in this case, we have:

$$\frac{\delta H}{\delta \rho}\,\delta\rho = 0, \qquad \frac{\delta^2 H}{\delta \rho^2}\,(\delta\rho, \delta\rho) = \frac{h'(\alpha_\ell) - h'(\alpha_r)}{\alpha_\ell - \alpha_r}\,(|\delta\rho_{\ell r}|^2 + |\delta\rho_{r\ell}|^2).$$

(iii) $\ell \neq r$ and $\alpha_\ell = \alpha_r = \alpha$. Then,

$$\alpha_\ell(t) = \alpha + |t\theta|/2, \qquad \alpha_r(t) = \alpha - |t\theta|/2.$$

It follows that

$$h(\alpha_\ell(t)) + h(\alpha_r(t)) = 2h(\alpha) + \frac{t^2\theta^2}{4}\,h''(\alpha) + o(t^2).$$

Then, we deduce that:

$$\frac{\delta H}{\delta \rho}\,\delta\rho = 0, \qquad \frac{\delta^2 H}{\delta \rho^2}\,(\delta\rho, \delta\rho) = h''(\alpha)(|\delta\rho_{\ell r}|^2 + |\delta\rho_{r\ell}|^2).$$

Collecting the results in the above three cases, leads to formulae (3.14) and (3.15). ▌

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