

# Quantum Maximum Entropy Principle and the Moments of the Generalized Wigner Function

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**Abstract.** By introducing a quantum entropy functional of the reduced density matrix, we construct a rigorous scheme to develop quantum hydrodynamic models. The principle of quantum maximum entropy permits to solve the closure problem for a quantum hydrodynamic set of balance equations corresponding to an arbitrary number of moments in the framework of extended thermodynamics. Quantum contributions are expressed in powers of  $\hbar^2$ .

## 1. Introduction

Hydrodynamical (HD) models are essential for a physical-mathematical description of the space-time evolution of any kind of fluids. For a rigorous derivation of an HD model the main difficulty is identified in the closure problem associated with the constraint that to solve a finite set of moment equations it is necessary the knowledge of higher order moments [1]. In classical mechanics, the introduction of a maximum entropy principle (MEP) has proven to be very fruitful in solving the closure problem to any degree of approximation [2]. In the quantum MEP (QMEP), the main issue is to define a proper quantum entropy for the explicit incorporation of statistics into problems involving a system of identical particles. The aim of this work is to address this issue and construct a complete set of quantum balance equations (QHD) which are rigorously closed within a global QMEP. Four main results are pointed out in the present paper.

## 2. The generalized Wigner equation, the QHD models and the QMEP approach

We consider a fixed number  $N$  of identical particles introducing the general Hamiltonian  $H = \int d^3r \Psi^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \Psi(\mathbf{r}) + \sum_{k=2}^L \frac{1}{k!} \int d^3r_1 \cdots \int d^3r_k \Psi^\dagger(\mathbf{r}_1) \cdots \Psi^\dagger(\mathbf{r}_k) V(\mathbf{r}_1, \dots, \mathbf{r}_k) \Psi(\mathbf{r}_k) \cdots \Psi(\mathbf{r}_1)$  in the Fock space, with many-body interactions and, the statistical density matrix  $\rho$ , being  $Tr(\rho) = 1$  and  $\Psi$  the particle field operator [3]. Analogously, in the coordinate space representation we can define the reduced density matrix [4] of single particle,  $\langle \mathbf{r} | \hat{\rho} | \mathbf{r}' \rangle = \langle \Psi^\dagger(\mathbf{r}') \Psi(\mathbf{r}) \rangle = Tr(\rho \Psi^\dagger(\mathbf{r}') \Psi(\mathbf{r}))$  that in an arbitrary representation will take the form  $\langle \nu | \hat{\rho} | \nu' \rangle = \langle a_\nu^\dagger, a_\nu \rangle = Tr(\rho a_\nu^\dagger, a_\nu)$  being  $\nu, \nu'$  single particle states,  $a_\nu, a_\nu^\dagger$  the annihilation and creation operators for these states,  $\langle \cdots \rangle$  the statistical mean value with  $Tr(\hat{\rho}) = N$ . Thus, we can define

[4] the *reduced* Wigner function

$$\mathcal{F}_{\mathcal{W}} = (2\pi\hbar)^{-3} \int d^3\tau e^{-\frac{i}{\hbar}\tau\cdot\mathbf{p}} \langle \Psi^\dagger(\mathbf{r} - \tau/2) \Psi(\mathbf{r} + \tau/2) \rangle \quad (1)$$

Accordingly, we look for a function  $\widetilde{\mathcal{M}}(\mathbf{r}, \mathbf{p})$  in phase space that *corresponds* unambiguously to a single particle operator  $\widehat{\mathcal{M}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$ , introducing the Weyl-Wigner transform  $\mathcal{W}(\widehat{\mathcal{M}}) = \widetilde{\mathcal{M}}$  and the inverse Weyl-Wigner transform  $\mathcal{W}^{-1}(\widetilde{\mathcal{M}}) = \langle \mathbf{r} | \widehat{\mathcal{M}} | \mathbf{r}' \rangle$ . Following an usual script [4, 5], we obtain the equation of motion for the *reduced Wigner function*

$$i\hbar \frac{\partial}{\partial t} \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}) = \int D\xi \left[ \widetilde{\mathcal{H}}(\mathbf{r}' + \tau/2, \mathbf{p}' + \phi/2) - \widetilde{\mathcal{H}}(\mathbf{r}' - \tau/2, \mathbf{p}' - \phi/2) \right] \mathcal{F}_{\mathcal{W}}(\mathbf{r}', \mathbf{p}') \quad (2)$$

where  $D\xi = d^3r' d^3p' d^3\tau d^3\phi e^{\frac{i}{\hbar}[\tau\cdot(\mathbf{p}' - \mathbf{p}) + \phi\cdot(\mathbf{r} - \mathbf{r}')]}$  and  $\widetilde{\mathcal{H}}$  the phase function of the single particle operator  $\widehat{\mathcal{H}} = \langle \mathcal{H} \rangle$ , being  $\mathcal{H} = -\hbar^2/2m\nabla^2 + V(\mathbf{r}) + \sum_{k=1}^{L-1} (1/k!) \int d^3r_1 \cdots \int d^3r_k \Psi^\dagger(\mathbf{r}_1) \cdots \Psi^\dagger(\mathbf{r}_k) V(\mathbf{r}, \mathbf{r}_1, \dots, \mathbf{r}_k) \Psi(\mathbf{r}_k) \cdots \Psi(\mathbf{r}_1)$ . Then, by expanding the integrand of (2) around  $\tau = 0$  and using the Fourier integral theorem, we obtain the formal full expansion, to all orders in  $\hbar$ , of the equation of motion for the *reduced Wigner function* in the generalized Hartree approximation [6]

$$\frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial t} + \frac{p_k}{m} \frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial x_k} = \sum_{l=0}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \left[ \frac{\partial^{2l+1} V_{eff}}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \right] \left[ \frac{\partial^{2l+1} \mathcal{F}_{\mathcal{W}}}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} \right] \quad (3)$$

where Einstein convention is used on the saturated indices, and the effects of interactions are entirely contained in the effective potential  $V_{eff}(\mathbf{r})$ . We remark that, if we do not describe in explicit way the many body interactions, then the expansion (3) will take only a formal value. As relevant application of this approach we consider a Bose gas with many-body contact interactions [7] and set  $V(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k) = c_{k-1} \prod_{i=1}^{k-1} \delta(\mathbf{r}_i - \mathbf{r}_{i+1})$  for  $\forall k \geq 2$ . In this case we have

$$V_{eff}(\mathbf{r}) = V(\mathbf{r}) + \sum_{k=1}^{L-1} \frac{c_k}{k!} g^{(k)}(\mathbf{r}) [n(\mathbf{r})]^k \quad \text{with} \quad g^{(k)}(\mathbf{r}) = \frac{\langle [\Psi^\dagger(\mathbf{r})]^k [\Psi(\mathbf{r})]^k \rangle}{[n(\mathbf{r})]^k} \quad (4)$$

where  $g^{(k)}(\mathbf{r})$  is the k-order correlation function [8]. We stress that, by considering explicitly the relation (4), then the kinetic equation (3) loses its formal value and, consequently, all non-linear phenomena imputable to weak interactions between bosons can be expressed in terms of increasing powers of density. The advantage of this approach will be evident in the corresponding QHD system. In this sense, a theory based on Eq. (3) supplemented by Eq. (4) is a first major result of the work, because all closure relations imputable to the contact interactions, are *explicitly determined* as known polynomial functions of the macroscopic field variable  $n(\mathbf{r})$  [9]. We remark that these results can be generalized by including explicitly the spin degrees of freedom. Equations (2),(3) can be supplemented by others interaction terms to describe a variety of physical systems, including Fermi liquids [5], non-ideal gases and plasma [10].

Below we develop the extended three-dimensional QHD model associated with (3). By considering the operator  $\widehat{\mathcal{M}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$  and the corresponding phase function  $\widetilde{\mathcal{M}}(\mathbf{r}, \mathbf{p})$  we define the macroscopic *local moment*  $M(\mathbf{r}, t) = \int d^3p \widetilde{\mathcal{M}}(\mathbf{r}, \mathbf{p}) \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}, t)$  of  $\widehat{\mathcal{M}}$ . As in classic extended thermodynamics [1], by introducing the group velocity  $u_i = p_i/m$ , we define the mean velocity  $v_i = n^{-1} \int d^3p u_i \mathcal{F}_{\mathcal{W}}$ , the peculiar velocity  $\tilde{u}_i = u_i - v_i$ , and the quantity  $\tilde{\varepsilon} = m\tilde{u}^2/2$ . Thus, we consider the set of traceless kinetic fields [11]  $\widetilde{\mathcal{M}}_A = \{\tilde{\varepsilon}^s, \tilde{\varepsilon}^s \tilde{u}_{i_1}, \dots, \tilde{\varepsilon}^s \tilde{u}_{\langle i_1} \tilde{u}_{i_2} \cdots \tilde{u}_{i_r} \rangle\}$  and the corresponding set of *central moments*  $M_A(\mathbf{r}, t) = \{M_{(s)}, M_{(s)|i_1}, \dots, M_{(s)|\langle i_1 \dots i_r \rangle}\}$  where, by construction, it is  $M_{(0)|i_1} = 0$ , and  $M_{(s)|\langle i_1 i_2 \dots i_r \rangle} = \int d^3p \tilde{\varepsilon}^s \tilde{u}_{\langle i_1} \tilde{u}_{i_2} \cdots \tilde{u}_{i_r} \rangle \mathcal{F}_{\mathcal{W}}$  with  $s = 0, 1, \dots, \mathcal{N}$  and  $r = 1, 2, \dots, M$ . In particular, by using a finite but arbitrary number of scalar and vectorial kinetic fields  $\widetilde{\mathcal{M}}_A = \{\tilde{\varepsilon}^s, \tilde{\varepsilon}^s \tilde{u}_i\}$  we obtain in correspondence the set of scalar and vectorial central moments  $M_A = \{M_{(s)}, M_{(s)|i}\}$  with  $s = 0, \dots, \mathcal{N}$ . Accordingly, for  $\mathcal{N} = 0$ , as set of macroscopic variables we get the *numerical density*  $n = M_{(0)}$  and the *velocity*  $v_i$ . For  $\mathcal{N} = 1$  we get in

addition  $M_{(1)}$  and  $M_{(1)|i}$ , which admit a direct physical interpretation being  $M_{(1)} = 3/2 P$  and  $M_{(1)|i} = q_i$  respectively, the *internal energy density* (with  $P$  the pressure) and the *heat flux density*. By contrast, for  $\mathcal{N} > 1$ , as macroscopic variables, we consider also some scalar and vectorial moments of higher order. Multiplying (3) by  $\widetilde{\mathcal{M}}_A$ , integrating over  $\mathbf{p}$  we exactly determine a theory that is consistent up to terms of order  $\hbar^2$ . Thus, the moments  $\{v_i, M_A\}$  must satisfy the following extended QHD<sub>2</sub> system

$$\dot{n} + n \frac{\partial v_k}{\partial x_k} = 0, \quad \dot{v}_i + \frac{1}{n} \frac{\partial M_{(0)|ik}}{\partial x_k} + \frac{1}{m} \frac{\partial V_{eff}}{\partial x_i} = 0, \tag{5}$$

$$\begin{aligned} \dot{M}_{(s)} + M_{(s)} \frac{\partial v_k}{\partial x_k} + \frac{\partial M_{(s)|k}}{\partial x_k} + s m M_{(s-1)|ik} \frac{\partial v_i}{\partial x_k} - s \frac{m}{n} M_{(s-1)|i} \frac{\partial M_{(0)|ik}}{\partial x_k} = \\ \frac{\hbar^2}{24} s(s-1) \left\{ (s-2) \frac{\partial^3 V_{eff}}{\partial x_{(i} \partial x_j \partial x_k)} M_{(s-3)|\langle ij k \rangle} + \frac{3(1+2s)}{5} \frac{\partial^3 V_{eff}}{\partial x_r \partial x_r \partial x_k} M_{(s-2)|k} \right\}, \end{aligned} \tag{6}$$

$$\begin{aligned} \dot{M}_{(s)|i} + M_{(s)|i} \frac{\partial v_k}{\partial x_k} + \frac{\partial M_{(s)|ik}}{\partial x_k} + s m M_{(s-1)|ijk} \frac{\partial v_j}{\partial x_k} + M_{(s)|k} \frac{\partial v_i}{\partial x_k} - \frac{M_{(s)}}{n} \frac{\partial M_{(0)|ik}}{\partial x_k} - \\ s m \frac{M_{(s-1)|ij}}{n} \frac{\partial M_{(0)|jk}}{\partial x_k} = \frac{\hbar^2}{24} s \left\{ (s-1)(s-2) \frac{\partial^3 V_{eff}}{\partial x_r \partial x_j \partial x_k} M_{(s-3)|\langle r j k i \rangle} + \right. \\ \left. \frac{3(s-1)}{m} \frac{(3+2s)}{7} \left( \frac{\partial^3 V_{eff}}{\partial x_r \partial x_r \partial x_k} M_{(s-2)|\langle k i \rangle} + \frac{\partial^3 V_{eff}}{\partial x_{\langle k} \partial x_r \rangle \partial x_i} M_{(s-2)|\langle k r \rangle} \right) + \right. \\ \left. \frac{(4s^2 + 8s + 3)}{5 m^2} \frac{\partial^3 V_{eff}}{\partial x_r \partial x_r \partial x_i} M_{(s-1)} \right\} \quad \text{with } s = 1, \dots, \mathcal{N}. \end{aligned} \tag{7}$$

The set (5) - (7) is a second major result of the work: in particular, for  $\hbar \rightarrow 0$ , it recovers the classic form of extended thermodynamics [1]. The set contains unknown constitutive functions that are represented by the central moments of higher order  $H_A = \{M_{N+1}, M_{(l)|\langle ij \rangle}, M_{(r)|\langle ijk \rangle}, M_{(s)|\langle ij qk \rangle}\}$  with  $l = 0, \dots, \mathcal{N}$ ;  $r = 0, \dots, \mathcal{N} - 1$ ; and  $s = 0, \dots, \mathcal{N} - 3$ .

In general, the closure problem of a set of balance equations is tackled using the QMEP formalism. Accordingly, to take into account *ab initio* the Bose and Fermi statistics, we follow the Landau strategy [12]. Thus, for a non-interacting system in non-equilibrium conditions, the quantum entropy can be determined in terms of the reduced density matrix  $\hat{\varrho}$  [13]. Then, by generalizing existing definitions [14], as quantum entropy we take the *global* quantity

$$S(\hat{\varrho}) = -k_B Tr(\hat{\Phi}(\hat{\varrho})) \quad \text{with} \quad \hat{\Phi}(\hat{\varrho}) = \hat{\varrho} \left\{ \ln \left( \frac{\hat{\varrho}}{y} \right) \pm y \hat{\varrho}^{-1} \left( \hat{I} \mp \frac{\hat{\varrho}}{y} \right) \ln \left( \hat{I} \mp \frac{\hat{\varrho}}{y} \right) \right\} \tag{8}$$

where  $k_B$  is the Boltzmann constant,  $\hat{I}$  is the identity operator,  $y = (2\tilde{s} + 1)$  is the spin degeneration and, the  $\pm$  signs refer to fermions and bosons, respectively. By using the QMEP, we search the extremal value of entropy subject to the constraint that the information on the physical system is described by the  $M_A(\mathbf{r}, t)$ . To this purpose, we consider the new *global* functional [15]

$$\tilde{S} = S - \int d^3r \left\{ \sum_{A=1}^{\mathcal{N}} \tilde{\lambda}_A \left[ \int d^3p \tilde{\mathcal{M}}_A \mathcal{F}_{\mathcal{W}} - M_A \right] \right\} \tag{9}$$

being  $\tilde{\lambda}_A(\mathbf{r}, t)$  the *local Lagrange multipliers* to be determined. One can show that  $\delta\tilde{S} = 0$  implies

$$\hat{\varrho} = y \left\{ \exp \left[ \mathcal{W}^{-1} \left( \sum_{A=1}^{\mathcal{N}} \lambda_A(\mathbf{r}, t) \tilde{\mathcal{M}}_A \right) \right] \pm \hat{I} \right\}^{-1} \tag{10}$$

with  $\lambda_A = \tilde{\lambda}_A/k_B$ . The (10) is a third major result of the work. We remark that, by using the (8), Bose or Fermi statistics are implicitly taken into account and, from relation (10), we obtain

$$\mathcal{F}_{\mathcal{W}} = (2\pi\hbar)^{-3} \mathcal{W} \left( \hat{\varrho}[\lambda_A(\mathbf{r}, t), \tilde{\mathcal{M}}_A] \right). \tag{11}$$

From the functional form (10)-(11) of the reduced Wigner function, we use the (3) to obtain a set of equations for the constraints. This set completely represents the closed QHD<sub>2</sub> model (5)-(7) in which all the constitutive functions are determined starting from their kinetic expressions. Thus, for a given number of moments  $M_A$ , we can consider a consistent expansion around  $\hbar$  of the Wigner function. In this way we separate classical from quantum dynamics, and obtain order by order corrections terms. In particular, by using the Moyal formalism, one can prove [16] that the Wigner function, and hence the central moments, can be expanded in even power of  $\hbar$  being  $\mathcal{F}_W = \sum_{k=0}^{\infty} \hbar^{2k} \mathcal{F}_W^{(2k)}$  and  $M_A = \sum_{k=0}^{\infty} \hbar^{2k} M_A^{(2k)}$ . With this approach, the dynamics of the system is described by resolving, order by order, a closed QHD set of balance equations for the moments  $\{M_A(\mathbf{r}, t)\}$ . To this end, the Lagrange multipliers  $\lambda_A$  are determined by inverting, order by order, the constraints  $M_A = (2\pi\hbar)^{-3} \int d^3p \widetilde{\mathcal{M}}_A \mathcal{W}(\widehat{q}[\lambda_B(\mathbf{r}, t), \widetilde{\mathcal{M}}_B])$  and the inversion problem can be solved only by assuming that also the Lagrange multipliers admit for an expansion in even powers of  $\hbar$ , i.e.  $\lambda_A = \lambda_A^{(0)} + \sum_{k=1}^{\infty} \hbar^{2k} \lambda_A^{(2k)}$ . With these assumptions, and using (10) and (11), we succeed in determining the following expression for  $\mathcal{F}_W$

$$\mathcal{F}_W = \frac{\widetilde{y}}{e^{\Pi} \pm 1} \left\{ 1 + \sum_{r=1}^{\infty} \hbar^{2r} P_{2r}^{\pm} \right\}, \quad (12)$$

where  $\widetilde{y} = y/(2\pi\hbar)^3$ ,  $\Pi = \sum \lambda_A \widetilde{\mathcal{M}}_A$  and the terms  $P_{2r}^{\pm}$  are expressed by recursive formulas.

The (12) is a fourth major result of the work. By considering terms up to first order in the quantum correction, the Lagrange multipliers are obtained as solutions of constraints  $M_A + \mathcal{O}(\hbar^4) = \int d^3p \widetilde{\mathcal{M}}_A \mathcal{F}_W$ . In this case,  $M_A$  must satisfy the QHD<sub>2</sub> system (5)-(7). From the knowledge of the Lagrange multipliers, both the Wigner function and the constitutive functions  $H_A$  can be determined explicitly. We remark that: (i) Using the general definition (8) we incorporate the indistinguishability principle of a system of identical particles, by developing a nonlocal theory that contains implicitly the Fermi and Bose statistics, a result which was left open since the Wigner seminal papers [16]. (ii) When  $\hbar \rightarrow 0$  we recover the expressions  $\lambda_A^{(0)} = \lambda_A^{(0)}(M_B^{(0)})$  and  $\mathcal{F}_W^{(0)}$  obtained in the framework of classic MEP approach [1] for a Fermions or Bosons system.

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- [11]  $A_{\langle i_1 \dots i_n \rangle}$  is the traceless symmetric part of tensor  $A_{i_1 \dots i_n}$  respect to indices contained between  $\langle \phantom{x} \rangle$ . Thus, for example, the quantity  $A_{\langle kr \rangle i}$  must be intended as it follows  $A_{\langle kr \rangle i} = (A_{kri} + A_{rki})/2 - 1/3 \delta_{kr} A_{lli}$ .
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