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Statistics and quantum maximum entropy principle

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Summary. — By using the *reduced* Wigner formalism we consider a kinetic theory for a quantum gas. We introduce a set of generalized kinetic fields and obtain a hierarchy of Quantum Hydrodynamic (QHD) equations for the corresponding macroscopic variables. To close the QHD system a maximum entropy principle is asserted, and to explicitly incorporate particles indistinguishability a proper quantum entropy is analyzed in terms of the reduced density matrix. This approach implies a quantum generalization of the corresponding Lagrange multipliers. Quantum contributions are expressed in powers of $\hbar^2$.

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1. – Introduction

The development of hydrodynamic (HD) approaches is of great interest from both an applied and theoretical fundamental point of view. In particular, to include the details of a microscopic description, different closure schemes can be implemented for the construction of self-consistent HD models [1, 2]. In classical mechanics, the introduction of a maximum entropy principle (MEP) proved to be very fruitful in solving the closure problem to any degree of approximation [2]. This is no longer the case in quantum mechanics, apart from some partial attempts [3-5]. In the quantum MEP (QMEP), the main difficulty rests on defining a proper quantum entropy for the explicit incorporation of statistics into problems involving a system of identical particles. Furthermore, also the quantum generalization of the corresponding Lagrange multipliers is an open problem. On the other hand, the availability of rigorous quantum HD (QHD) models is a demanding issue for a variety of quantum systems like interacting fermionic and bosonic gases, quantized vortices, quantum turbulence, confined carrier transport in semiconductor heterostructures, nuclear physics, etc.

The aim of this work is to expand the results known in the literature [3-5]. To this purpose, we define a suitable quantum entropy, in terms of the *reduced density matrix*, and incorporate the *indistinguishability principle* for a system of identical particles. As a consequence, we include explicitly both Fermi and Bose statistics in the framework of a non-local theory for the reduced Wigner function. We further determine a quantum-hydrodynamic system for an arbitrary set of scalar and vectorial central moments used as constraints in the QMEP approach. Finally, we develop a quantum closure procedure using a set of quantum Lagrange multipliers to determine the potentials associated with external constraints.

2. – The Wigner formalism, the QHD equations, the QMEP approach

We consider a given number N of identical particles and introduce, in Fock space, the statistical density matrix ρ with $\mathrm{Tr}(\rho) = 1$ (we suppress the symbol $\widehat{}$ to refer to operators acting in Fock space) and the standard Hamiltonian including many-body interactions,

$$H = \int \mathrm{d}^3 r\, \Psi^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2\,m} \nabla^2 + V(\mathbf{r}) \right] \Psi(\mathbf{r}) + \sum_{k=2}^{R} \frac{1}{k!} \int \mathrm{d}^3 r_1 \cdots \int \mathrm{d}^3 r_k \Psi^\dagger(\mathbf{r_1}) \cdots \Psi^\dagger(\mathbf{r_k})\, V(\mathbf{r_1}, \ldots, \mathbf{r_k}) \Psi(\mathbf{r_k}) \cdots \Psi(\mathbf{r_1}), \tag{1}$$

where m is the quasi-particle effective mass and, neglecting the spin degree of freedom, Ψ is the particle field operator. Analogously, in the coordinate space representation we define the reduced density matrix [6] of single particle $\langle \mathbf{r} | \widehat{\varrho} | \mathbf{r'} \rangle = \langle \Psi^\dagger(\mathbf{r'}) \Psi(\mathbf{r}) \rangle = \mathrm{Tr}(\rho \Psi^\dagger(\mathbf{r'}) \Psi(\mathbf{r}))$ that in an arbitrary representation takes the form $\langle \boldsymbol{\nu} | \widehat{\varrho} | \boldsymbol{\nu'} \rangle = \langle a^\dagger_{\nu'} a_\nu \rangle = \mathrm{Tr}(\rho\, a^\dagger_{\nu'} a_\nu)$, ν, ν' being single particle states, a_ν, $a^\dagger_{\nu'}$ the annihilation and creation operators for these states and $\langle \cdots \rangle$ the statistical mean value. By using this formalism [6-8], we define the *reduced* Wigner function

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

obtaining for the momentum space distribution function $\int \mathrm{d}^3 r \mathcal{F}_\mathcal{W} = \langle a^\dagger_p a_p \rangle = \langle N_p \rangle$ and, analogously, the dual expression $\int \mathrm{d}^3 p\, \mathcal{F}_\mathcal{W} = \langle \Psi^\dagger(\mathbf{r})\, \Psi(\mathbf{r}) \rangle = n(\mathbf{r})$, where $\langle N_p \rangle$ is the mean occupation number, $n(\mathbf{r})$ is the quasi-particle numerical density, with $\mathrm{Tr}(\widehat{\varrho}) = N$. Accordingly, we look [9] for a function $\widetilde{\mathcal{M}}(\mathbf{r}, \mathbf{p})$ in phase space that *corresponds* unambiguously to an operator of single particle $\widehat{\mathcal{M}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$, introducing the Weyl-Wigner transform $\mathcal{W}(\widehat{\mathcal{M}}) = \widetilde{\mathcal{M}}(\mathbf{r}, \mathbf{p}) = \int \mathrm{d}^3 \tau\ \langle \mathbf{r} + \boldsymbol{\tau}/2 \,|\, \widehat{\mathcal{M}} \,|\, \mathbf{r} - \boldsymbol{\tau}/2 \rangle\ e^{-\frac{i}{\hbar} \boldsymbol{\tau} \cdot \mathbf{p}}$. Analogously, we define the inverse Weyl-Wigner transform $\mathcal{W}^{-1}(\widetilde{\mathcal{M}}) = \langle \mathbf{r} | \widehat{\mathcal{M}} | \mathbf{r'} \rangle = (2\pi\hbar)^{-3} \int \mathrm{d}^3 p\ \widetilde{\mathcal{M}}((\mathbf{r} + \mathbf{r'})/2, \mathbf{p})\ e^{\frac{i}{\hbar} \mathbf{p} \cdot (\mathbf{r} - \mathbf{r'})}$. Thus, $\widetilde{\varrho}(\mathbf{r}, \mathbf{p}) = \mathcal{W}(\widehat{\varrho}) = (2\pi\hbar)^3\, \mathcal{F}_\mathcal{W}(\mathbf{r}, \mathbf{p})$ and $\langle \mathbf{r} | \widehat{\varrho} | \mathbf{r'} \rangle = \mathcal{W}^{-1}(\widetilde{\varrho})$. Following a usual script, in the generalized Hartree approximation, the equation of motion for the *reduced Wigner function* takes the compact form

$$i\hbar \frac{\partial}{\partial t} \mathcal{F}_\mathcal{W}(\mathbf{r}, \mathbf{p}) = \int \mathrm{D}\xi \left[\widetilde{\mathcal{H}} \left(\mathbf{r'} + \frac{\boldsymbol{\tau}}{2}, \mathbf{p'} + \frac{\boldsymbol{\phi}}{2} \right) - \widetilde{\mathcal{H}} \left(\mathbf{r'} - \frac{\boldsymbol{\tau}}{2}, \mathbf{p'} - \frac{\boldsymbol{\phi}}{2} \right) \right] \mathcal{F}_\mathcal{W}(\mathbf{r'}, \mathbf{p'}), \tag{3}$$

where $\mathrm{D}\xi = \mathrm{d}^3 r' \mathrm{d}^3 p' \mathrm{d}^3 \tau \mathrm{d}^3 \phi\, e^{\frac{i}{\hbar} [\boldsymbol{\tau} \cdot (\mathbf{p'} - \mathbf{p}) + \boldsymbol{\phi} \cdot (\mathbf{r} - \mathbf{r'})]}$ and $\widetilde{\mathcal{H}}$ is the phase function of single-particle operator $\widehat{\mathcal{H}} = \langle \mathcal{H} \rangle$ being $\mathcal{H} = -\hbar^2/2m\nabla^2 + V(\mathbf{r}) + \sum_{k=1}^{R-1} (1/k!) \int \mathrm{d}^3 r_1 \cdots \int \mathrm{d}^3 r_k\ \Psi^\dagger(\mathbf{r_1}) \cdots \Psi^\dagger(\mathbf{r_k}) V(\mathbf{r}, \mathbf{r_1}, \ldots, \mathbf{r_k}) \Psi(\mathbf{r_k}) \cdots \Psi(\mathbf{r_1})$.

Without loss of generality, it is possible to expand the integrand of eq. (3) as a McLaurin series around $\boldsymbol{\tau} = 0$. Thus, by using the Fourier integral theorem, we obtain the full gradient expansion to all orders in $\hbar$, in the generalized Hartree approximation [10,11]

$$(4) \qquad \frac{\partial \mathcal{F}_\mathcal{W}}{\partial t} = -\frac{p_k}{m}\frac{\partial \mathcal{F}_\mathcal{W}}{\partial x_k} + \sum_{l=0}^{\infty} \frac{(i\,\hbar/2)^{2l}}{(2l+1)!}\left[\frac{\partial^{2l+1} V_{\text{eff}}}{\partial x_{k_1}\cdots\partial x_{k_{2l+1}}}\right]\left[\frac{\partial^{2l+1}\mathcal{F}_\mathcal{W}}{\partial p_{k_1}\cdots\partial p_{k_{2l+1}}}\right],$$

where Einstein convention is used on the saturated indices and the effects of interactions are entirely contained in the definition of $V_{\text{eff}}(\mathbf{r})$.

As relevant application of this approach we consider a Bose gas with many-body contact interactions [12] and set $V(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_k}) = c_{k-1}\prod_{i=1}^{k-1}\delta(\mathbf{r_i} - \mathbf{r_{i+1}})$ for $\forall\, k \geq 2$ to obtain

$$(5) \qquad V_{\text{eff}}(\mathbf{r}) = V(\mathbf{r}) + \sum_{k=1}^{R-1}\frac{c_k}{k!}\, g^{(k)}(\mathbf{r})\,[n(\mathbf{r})]^k,$$

where $g^{(k)}(\mathbf{r}) = \langle[\Psi^\dagger(\mathbf{r})]^k[\Psi(\mathbf{r})]^k\rangle/[n(\mathbf{r})]^k$ is the k-order correlation function [13]. We stress that, by considering the explicit relation (5), the kinetic equation (4) 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. Indeed, all closure relations imputable to contact interactions are *explicitly determined* as known polynomial functions of the field variable $n(\mathbf{r})$. In this sense, a theory based on eqs. (4) and (5) is a first major result of the work because it can be applied to describe the same approximations governed by a generalized Gross-Pitaevskii equation (see Appendix A).

The above results can be formulated by including explicitly the spin degrees of freedom and eqs. (3), (4) can be supplemented by other interaction terms. In this way the theory can be used for a variety of physical systems, including metals, Fermi liquids [7], non-ideal gases and plasmas [14].

Below, we develop the extended QHD model associated with (4). We further express the leading-order correction to the classical models within an expansion in powers of order $\hbar^2$, hereafter labeled as QHD$_2$. By recalling that the expectation value of $\widehat{\mathcal{M}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$ can be expressed by the *global* quantity $\langle\widehat{\mathcal{M}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})\rangle = \int\int \mathrm{d}^3p\, \mathrm{d}^3r\, \widetilde{\mathcal{M}}(\mathbf{r}, \mathbf{p})\, \mathcal{F}_\mathcal{W}(\mathbf{r}, \mathbf{p}, t)$, we define the macroscopic *local moment* M of $\widehat{\mathcal{M}}$ by means of the *local* relations $M(\mathbf{r}, t) = \int \mathrm{d}^3p\, \widetilde{\mathcal{M}}(\mathbf{r}, \mathbf{p})\, \mathcal{F}_\mathcal{W}(\mathbf{r}, \mathbf{p}, t)$. As in classic extended thermodynamics [1], by introducing the group velocity $u_i = p_i/m$, we define the mean velocity $v_i = n^{-1}\int \mathrm{d}^3p\, u_i\, \mathcal{F}_\mathcal{W}$, the peculiar velocity $\widetilde{u}_i = u_i - v_i$, and the quantity $\widetilde{\varepsilon} = m\widetilde{u}^2/2$. Thus, we consider the set of traceless kinetic fields $\widetilde{\mathcal{M}}_A = \{\widetilde{\varepsilon}^s, \widetilde{\varepsilon}^s\widetilde{u}_{i_1}, \ldots, \widetilde{\varepsilon}^s\widetilde{u}_{\langle i_1}\,\widetilde{u}_{i_2}\cdots\widetilde{u}_{i_r\rangle}\}$ and the corresponding set of *central moments* $M_A(\mathbf{r}, t) = \{M_{(s)}, M_{(s)|i_1}, \ldots, M_{(s)|\langle i_1\cdots i_r\rangle}\}$ (where with $A_{\langle i_1\cdots i_n\rangle}$ we indicate the traceless symmetric part of tensor $A_{i_1\cdots i_n}$) being, by construction, $M_{(0)|i_1} = 0$, and

$$(6) \qquad M_{(s)|\langle i_1 i_2\cdots i_r\rangle} = \int \mathrm{d}^3p\, \widetilde{\varepsilon}^s\, \widetilde{u}_{\langle i_1}\,\widetilde{u}_{i_2}\cdots\widetilde{u}_{i_r\rangle}\, \mathcal{F}_\mathcal{W}$$

with $s = 0, 1, \ldots \mathcal{N}$ and $r = 1, 2, \ldots M$. In particular, by using a finite but arbitrary number of scalar and vectorial kinetic fields $\widetilde{\mathcal{M}}_A = \{\widetilde{\varepsilon}^s, \widetilde{\varepsilon}^s\widetilde{u}_i\}$ we obtain in correspondence the set of scalar and vectorial central moments $M_A = \{M_{(s)}, M_{(s)|i}\}$, with $s = 0, \cdots \mathcal{N}$.

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 eq. (4) by $\widetilde{\mathcal{M}}_A$, integrating over $\mathbf{p}$ we exactly determine the corresponding set of quantum balance equations to all orders in $\hbar$. In particular, following this approach, we can formulate a theory that is consistent up to the first quantum correction. Thus, the moments $\{v_i, M_A\}$ must satisfy the extended QHD system up to terms of order $\hbar^2$ (QHD$_2$) and we have the following balance equations:

$$\text{(7)}\quad \dot{n} + n\,\frac{\partial v_k}{\partial x_k} = 0\,, \qquad \dot{v}_i + \frac{1}{n}\,\frac{\partial M_{(0)|ik}}{\partial x_k} + \frac{1}{m}\,\frac{\partial V_{\text{eff}}}{\partial x_i} = 0,$$

$$\text{(8)}\quad \dot{M}_{(s)} + M_{(s)}\,\frac{\partial v_k}{\partial x_k} + \frac{\partial M_{(s)|k}}{\partial x_k} + s\,m\,M_{(s-1)|ik}\,\frac{\partial v_i}{\partial x_k} - s\frac{m}{n}\,M_{(s-1)|i}\,\frac{\partial M_{(0)|ik}}{\partial x_k} = \frac{\hbar^2}{24}\,s(s-1)\left\{(s-2)\,\frac{\partial^3 V_{\text{eff}}}{\partial x_{\langle i}\partial x_j \partial x_{k\rangle}}\,M_{(s-3)|\langle ijk\rangle} + \frac{3}{5}\frac{(1+2s)}{m}\,\frac{\partial^3 V_{\text{eff}}}{\partial x_r \partial x_r \partial x_k}\,M_{(s-2)|k}\right\},$$

$$\text{(9)}\quad \dot{M}_{(s)|i} + M_{(s)|i}\frac{\partial v_k}{\partial x_k} + \frac{\partial M_{(s)|ik}}{\partial x_k} + smM_{(s-1)|ijk}\frac{\partial v_j}{\partial x_k} - \frac{M_{(s)}}{n}\,\frac{\partial M_{(0)|ik}}{\partial x_k} + M_{(s)|k}\frac{\partial v_i}{\partial x_k} - sm\frac{M_{(s-1)|ij}}{n}\,\frac{\partial M_{(0)|jk}}{\partial x_k} = \frac{\hbar^2}{24}\,s\left\{(s-1)(s-2)\,\frac{\partial^3 V_{\text{eff}}}{\partial x_r \partial x_j \partial x_k}M_{(s-3)|\langle rjki\rangle} + \frac{3(s-1)}{m}\,\frac{(3+2s)}{7}\left(\frac{\partial^3 V_{\text{eff}}}{\partial x_r \partial x_r \partial x_k}\,M_{(s-2)|\langle ki\rangle} + \frac{\partial^3 V_{\text{eff}}}{\partial x_{\langle k}\partial x_{r\rangle}\partial x_i}\,M_{(s-2)|\langle kr\rangle}\right) + \frac{(4s^2+8s+3)}{5\,m^2}\,\frac{\partial^3 V_{\text{eff}}}{\partial x_r \partial x_r \partial x_i}\,M_{(s-1)}\right\} \qquad \text{with} \qquad s = 1, \cdots \mathcal{N},$$

where one has to take $M_{(l)|i_1 \cdots i_r} = 0$ if $l < 0$. The set of balance equations (7)-(9) is a second major result of the work and, for $\hbar \to 0$, it recovers the classic form of extended thermodynamics [1, 15]. The previous set of equations contains unknown constitutive functions which are represented by the central moments of higher order $H_A = \{M_{\mathcal{N}+1}, M_{(l)|\langle ij\rangle}, M_{(r)|\langle ijk\rangle}, M_{(p)|\langle ijqk\rangle}\}$ with $l = 0, \cdots \mathcal{N}$; $r = 0, \cdots \mathcal{N} - 1$; and $p = 0, \cdots \mathcal{N} - 3$.

In general, the closure problem of a set of balance equations is tackled using the QMEP formalism [3-5]. Accordingly, to take into account *ab initio* the statistics for a system of identical particles, we follow the Landau strategy [16] by evaluating the entropy as the logarithm of *statistical weight*. Thus, for a non-interacting system of fermions or bosons, in non-equilibrium conditions, the quantum entropy can be determined in terms of the mean occupation numbers in the form $S = -k_B \sum_\nu y[\langle \overline{N_\nu}\rangle \ln \langle \overline{N_\nu}\rangle \pm (1 \mp \langle \overline{N_\nu}\rangle) \ln(1 \mp \langle \overline{N_\nu}\rangle)]$ with k_B the Boltzmann constant, $\langle \overline{N_\nu}\rangle = \langle a_\nu^\dagger a_\nu\rangle / y$, and $y = (2\tilde{s} + 1)$ the spin degeneration where the upper and lower signs refer to fermions and bosons, respectively. If we consider the Schrodinger equation of single particle $[\widehat{\mathcal{H}}(\mathbf{r}) - E_\nu]\varphi_\nu(\mathbf{r}) = 0$, then, under stationary conditions, both the reduced density matrix $\widehat{\varrho}$ and any operator $\widehat{\Phi}(\widehat{\varrho})$ are diagonal in the base φ_ν. Thus, by introducing as a function of $\widehat{\varrho}$ the following quantity:

$$\text{(10)}\qquad \widehat{\Phi}(\widehat{\varrho}) = \widehat{\varrho}\left\{\ln\left(\frac{\widehat{\varrho}}{y}\right) \pm y\,\widehat{\varrho}^{-1}\left(\widehat{I} \mp \frac{\widehat{\varrho}}{y}\right)\ln\left(\widehat{I} \mp \frac{\widehat{\varrho}}{y}\right)\right\}$$

with $\widehat{I}$ the identity, we obtain $\langle \boldsymbol{\nu}|\widehat{\varrho}|\boldsymbol{\nu}'\rangle = \langle a_\nu^\dagger a_\nu\rangle\, \delta_{\nu\nu'}$ and $\langle \boldsymbol{\nu}|\widehat{\Phi}(\widehat{\varrho})|\boldsymbol{\nu}'\rangle = y[\langle \overline{N_\nu}\rangle \ln \langle \overline{N_\nu}\rangle \pm (1 \mp \langle \overline{N_\nu}\rangle) \ln(1 \mp \langle \overline{N_\nu}\rangle)]\, \delta_{\nu\nu'}$. As a consequence, by generalizing existing definitions [3-5, 17-19], Bose or Fermi statistics can be implicitly taken into account by defining the quantum entropy, for the whole system, in terms of the functional

$$S(\widehat{\varrho}) = -k_B \,\mathrm{Tr}(\widehat{\Phi}(\widehat{\varrho})) \tag{11}$$

with $\widehat{\Phi}(\widehat{\varrho})$ given by eq. (10).

To develop the QMEP approach in phase space, by rewriting eq. (11) as $S(\widehat{\varrho}) = -k_B\,(2\pi\hbar)^{-3}\int\int \mathrm{d}^3p\,\mathrm{d}^3r\,\mathcal{W}(\widehat{\Phi})$ we introduce the corresponding phase function $\widetilde{\Phi}(\mathbf{r},\mathbf{p}) = \mathcal{W}(\widehat{\Phi})$, and search the extremal value of entropy subject to the constraint that the accessible information on the physical system is described by the set $\{M_A(\mathbf{r},t)\}$. To this purpose, we consider the new *global* functional

$$\widetilde{S} = S - \int \mathrm{d}^3r \left\{ \sum_{A=1}^{\mathrm{N}} \widetilde{\lambda}_A \left[\int \mathrm{d}^3p\, \widetilde{\mathcal{M}}_A\, \mathcal{F}_{\mathcal{W}} - M_A \right] \right\}, \tag{12}$$

$\widetilde{\lambda}_A = \widetilde{\lambda}_A(\mathbf{r},t)$ being the *local Lagrange multipliers* to be determined. It is possible to show that the solution of the constraint $\delta\widetilde{S} = 0$ implies

$$\widehat{\varrho} = y \left\{ \exp\left[\mathcal{W}^{-1}\left(\sum_{A=1}^{\mathrm{N}} \lambda_A(\mathbf{r},t)\, \widetilde{\mathcal{M}}_A \right)\right] \pm \widehat{I} \right\}^{-1} \tag{13}$$

with $\lambda_A = \widetilde{\lambda}_A/k_B$.

Equation (13) is a third major result of the work. We remark that, by using eq. (10), Bose or Fermi statistics are implicitly taken into account. Thus, from eq. (13) the reduced Wigner function takes the form

$$\mathcal{F}_{\mathcal{W}} = \frac{1}{(2\pi\hbar)^3}\, \mathcal{W}\left(\widehat{\varrho}[\lambda_A(\mathbf{r},\, t), \widetilde{\mathcal{M}}_A] \right). \tag{14}$$

We stress that, in the set of hydrodynamic equations (7)-(9), the effects of interactions are entirely contained in $V_{\text{eff}}(\mathbf{r})$. Then, to take into account the detailed kinetics of the interactions, we consider the above approach in a dynamical context. Indeed, as in the classical case [2], by itself the QMEP does not provide any information about the dynamic evolution of the system, but offers only a definite procedure for the construction of a sequence of approximations for the non-equilibrium Wigner function. To obtain a dynamical description, it is necessary: i) to know a set of evolution equations for the constraints that includes the microscopic kinetic details, ii) to determine the Lagrange multipliers in terms of these constraints. In this way, the QMEP approach implicitly includes all the kinetic details of the microscopic interactions between particles. From the knoweledge of the functional form (13), (14) of the reduced Wigner function, we use eq. (4) to obtain a set of equations for the constraints. This set completely represents the closed QHD_2 model (7)-(9) in which all the constitutive functions are determined starting from their kinetic expressions. Accordingly, for a given number of moments M_A, we can consider a consistent expansion in powers of $\hbar$ 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 [20-22] that the Wigner function, and hence the central moments, can be expanded in even power of $\hbar$

$$\mathcal{F}_{\mathcal{W}} = \sum_{k=0}^{\infty} \hbar^{2k}\, \mathcal{F}_{\mathcal{W}}^{(2k)}\,, \quad M_A = \sum_{k=0}^{\infty} \hbar^{2k}\, M_A^{(2k)}. \tag{15}$$

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 λ_A must be determined by inverting, order by order, the constraints

$$M_A = \frac{1}{(2\pi\hbar)^3} \int \mathrm{d}^3 p\, \widetilde{\mathcal{M}}_A\, \mathcal{W}\left(\widehat{\varrho}[\lambda_B(\mathbf{r},\, t), \widetilde{\mathcal{M}}_B]\right). \tag{16}$$

The inversion problem can be solved only by assuming that also the Lagrange multipliers admit for an expansion in even powers of $\hbar$

$$\lambda_A = \lambda_A^{(0)} + \sum_{k=1}^{\infty} \hbar^{2k}\, \lambda_A^{(2k)}\,. \tag{17}$$

With these assumptions, and using eq. (13) and eq. (14), we succeed in determining the following expression for $\mathcal{F}_{\mathcal{W}}$:

$$\mathcal{F}_{\mathcal{W}} = \frac{\widetilde{y}}{e^{\Pi} \pm 1} \left\{ 1 + \sum_{r=1}^{\infty} \hbar^{2r} P_{2r}^{\pm} \right\}, \tag{18}$$

where $\widetilde{y} = y/(2\pi\hbar)^3$, $\Pi = \sum \lambda_A\, \widetilde{\mathcal{M}}_A$ and the nonlocal terms $P_{2r}^{\pm}$ are expressed by recursive formulae (as an example, for $r = 1$, the term $P_2^{\pm}$ is reported in Appendix B).

Equation (18) 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 eq. (16). In this case, M_A must satisfy the QHD$_2$ system (7)-(9). From the knowledge of the Lagrange multipliers, both the Wigner function and the constitutive functions H_A can be determined explicitly. In this respect we remark that: i) In the limit $\hbar \to 0$ we obtain that $\lambda_A \to \lambda_A^{(0)}$ and $\mathcal{F}_{\mathcal{W}} \to \mathcal{F}_{\mathcal{W}}^{(0)}$ where $\lambda_A^{(0)} = \lambda_A^{(0)}(M_B^{(0)})$ and $\mathcal{F}_{\mathcal{W}}^{(0)}$ recover the expressions for both the Lagrange multipliers and the distribution function obtained in the framework of the classic MEP approach [1]. ii) In local equilibrium conditions we obtain the Maxwell-Boltzmann distribution function for nondegenerate gases, and the Bose or Fermi distribution functions for degenerate gases, a result which was left open since the Wigner seminal papers [20, 21].

We conclude by remarking that this approach could be further generalized, to develop a non-local theory, also in fractional statistics. In this case, the entropy of the system should be expressed in terms of the logarithm of the *statistical weight* introduced by Wu [23] and the QMEP should be developed in terms of the reduced density matrix for particles obeying fractional exclusion statistics.

Appendix A.

We consider the generalized Gross-Pitaevskii equation with nonlinear terms of the odd type

$$i\hbar \frac{\partial \varphi(\mathbf{r},t)}{\partial t} = \langle \mathbf{r}|\widehat{H}_L|\varphi\rangle + \sum_{j=1}^{R-1} \mathrm{u}_j \, |\varphi(\mathbf{r},t)|^{2j} \, \varphi(\mathbf{r},t), \tag{A.1}$$

where $R \geq 2$, $\widehat{H}_L = \widehat{p}^2/2m + \widehat{V}$ describes the linear dynamics and u_j describe a many-body interaction within the mean-field approximation. By introducing the reduced Wigner function in term of wave function $\varphi(\mathbf{r},t)$, we obtain $\mathcal{F}_{\mathcal{W}} = (2\pi\hbar)^{-3} \int \mathrm{d}^3\tau \, e^{-\frac{i}{\hbar}\boldsymbol{\tau}\cdot\mathbf{p}} \; \varphi^*(\mathbf{r}-\boldsymbol{\tau}/2,t)\,\varphi(\mathbf{r}+\boldsymbol{\tau}/2,t)$. To obtain the *generalized Wigner equation* we calculate

$$\frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial t} = \frac{1}{(2\pi\hbar)^3} \int \mathrm{d}^3\tau \, e^{-\frac{i}{\hbar}\boldsymbol{\tau}\cdot\mathbf{p}} \left[\frac{\partial \varphi^*(\mathbf{r}-\boldsymbol{\tau}/2,t)}{\partial t} \right. \\ \left. \times \varphi(\mathbf{r}+\boldsymbol{\tau}/2,t) + \varphi^*(\mathbf{r}-\boldsymbol{\tau}/2,t)\, \frac{\partial \varphi(\mathbf{r}+\boldsymbol{\tau}/2,t)}{\partial t} \right] \tag{A.2}$$

and using eq. (A.1) we have $\partial\varphi/\partial t = \partial\varphi/\partial t|_L + \partial\varphi/\partial t|_{NL}$, where $\partial\varphi/\partial t|_L = \langle \mathbf{r}|\widehat{H}_L|\varphi\rangle/i\hbar$ describes the single particle linear dynamics, while the nonlinear part is expressed by

$$\left.\frac{\partial \varphi}{\partial t}\right|_{\mathrm{NL}} = \frac{1}{i\hbar} \sum_{j=1}^{R-1} \mathrm{u}_j |\varphi(\mathbf{r},t)|^{2j} \, \varphi(\mathbf{r},t). \tag{A.3}$$

By inserting the term $\partial\varphi/\partial t|_L$ in eq. (A.2) we describe the single-particle linear dynamics. Thus, we have the linear part $\partial\mathcal{F}_{\mathcal{W}}/\partial t|_L$ expressed by an expansion analogous to relation (4) where V_{eff} is replaced by the potential $V(\mathbf{r})$. Analogously, by inserting eq. (A.3) in eq. (A.2) we obtain the term which describes the nonlinear dynamics

$$\left.\frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial t}\right|_{\mathrm{NL}} = \frac{i/\hbar}{(2\pi\hbar)^3} \sum_{j=1}^{R-1} \mathrm{u}_j \int \mathrm{d}^3\tau e^{-\frac{i}{\hbar}\boldsymbol{\tau}\cdot\mathbf{p}} \left[F_j(\mathbf{r}-\boldsymbol{\tau}/2,t) - F_j(\mathbf{r}+\boldsymbol{\tau}/2,t)\right] \\ \times \int \mathrm{d}^3p' e^{\frac{i}{\hbar}\boldsymbol{\tau}\cdot\mathbf{p}'} \mathcal{F}_{\mathcal{W}}(\mathbf{r},\mathbf{p}')$$

with $\varphi^*(\mathbf{r}-\boldsymbol{\tau}/2,\,t)\,\varphi(\mathbf{r}+\boldsymbol{\tau}/2,\,t) = \int \mathrm{d}^3p' e^{\frac{i}{\hbar}\boldsymbol{\tau}\cdot\mathbf{p}'} \mathcal{F}_{\mathcal{W}}(\mathbf{r},\mathbf{p}',t)$ and $F_j(\mathbf{r}\pm\boldsymbol{\tau}/2,\,t) = |\varphi(\mathbf{r}\pm\boldsymbol{\tau}/2,\,t)|^{2j}$. By expanding $F_j(\mathbf{r}\pm\boldsymbol{\tau}/2,\,t)$ in series around $\boldsymbol{\tau} = 0$ and considering the following relation (where use is made of the property that $\mathcal{F}_{\mathcal{W}}$ and all derivatives of $\mathcal{F}_{\mathcal{W}}$

vanish for $\mathbf{r}, \mathbf{p} \to \infty$):

$$-\frac{\partial^{2l+1} F_j(\mathbf{r},\, t)}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \int \mathrm{d}^3 p' \, \frac{\partial^{2l+1} e^{\frac{i}{\hbar}\boldsymbol{\tau}\cdot\mathbf{p}'}}{\partial p'_{k_1} \cdots \partial p'_{k_{2l+1}}} \mathcal{F}_{\mathcal{W}} =$$
$$\frac{\partial^{2l+1} F_j(\mathbf{r},\, t)}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \int \mathrm{d}^3 p' \frac{\partial^{2l+1} \mathcal{F}_{\mathcal{W}}}{\partial p'_{k_1} \cdots \partial p'_{k_{2l+1}}} \, e^{\frac{i}{\hbar}\boldsymbol{\tau}\cdot\mathbf{p}'}$$

we find

$$\text{(A.4)} \qquad \left.\frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial t}\right|_{\mathrm{NL}} = \frac{1}{(2\pi\hbar)^3} \sum_{j=1}^{R-1} \mathrm{u}_j \sum_{l=0}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \int \mathrm{d}^3\tau e^{-\frac{i}{\hbar}\boldsymbol{\tau}\cdot\mathbf{p}} \times \left\{ \frac{\partial^{2l+1} F_j(\mathbf{r},\, t)}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \int \mathrm{d}^3 p' \, \frac{\partial^{2l+1} \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}', t)}{\partial p'_{k_1} \cdots \partial p'_{k_{2l+1}}} \, e^{\frac{i}{\hbar}\boldsymbol{\tau}\cdot\mathbf{p}'} \right\}.$$

Thus, by using the Fourier integral theorem, the nonlinear contribute (A.4) takes the following form:

$$\text{(A.5)} \qquad \left.\frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial t}\right|_{\mathrm{NL}} = \sum_{l=0}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \left\{ \frac{\partial^{2l+1} \sum_{j=1}^{R-1} \mathrm{u}_j \, [n(\mathbf{r},\, t)]^j}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \right\} \left\{ \frac{\partial^{2l+1} \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}, t)}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} \right\},$$

where use is made of the property $F_j(\mathbf{r}, t) = [n(\mathbf{r}, t)]^j$.

Being $\partial \mathcal{F}_{\mathcal{W}}/\partial t = \partial \mathcal{F}_{\mathcal{W}}/\partial t|_L + \partial \mathcal{F}_{\mathcal{W}}/\partial t|_{NL}$, the full gradient expansion of the Wigner equation will take the form reported in eq. (4) to all order of $\hbar$, with

$$\text{(A.6)} \qquad V_{\mathrm{eff}}(\mathbf{r}) = V(\mathbf{r}) + \sum_{k=1}^{R-1} \mathrm{u}_k \, [n(\mathbf{r})]^k.$$

We remark that for $R = 2$ (Gross-Pitaevskii equation) relation (A.6) coincides exactly with eq. (5). Analogously, by considering eq. (5) for $R > 2$, a reasonable description of the low-energy dynamics can be given by assuming values approximatively constant for the remaining correlation functions (see § 7.6, in [13]). Thus, also in this case eq. (A.6) can be determined as a particular case of eq. (5).

Appendix B.

By considering explicitly the first term of expansion (18) we have

$$P_2^{\pm} = -\left(\frac{e^{\Pi_0}}{e^{\Pi_0} \pm 1} \right) [\mathcal{H}_3 + \mathcal{H}_2] + 2 \left(\frac{e^{\Pi_0}}{e^{\Pi_0} \pm 1} \right)^2 [3\,\mathcal{H}_3 + \mathcal{H}_2] - 6 \left(\frac{e^{\Pi_0}}{e^{\Pi_0} \pm 1} \right)^3 \mathcal{H}_3,$$

where

$$\mathcal{H}_3 = -\frac{1}{24} \left[\frac{\partial^2 \Pi_0}{\partial x_i \partial x_j} \frac{\partial \Pi_0}{\partial p_i} \frac{\partial \Pi_0}{\partial p_j} + \frac{\partial^2 \Pi_0}{\partial p_i \partial p_j} \frac{\partial \Pi_0}{\partial x_i} \frac{\partial \Pi_0}{\partial x_j} - 2 \, \frac{\partial^2 \Pi_0}{\partial x_i \partial p_j} \frac{\partial \Pi_0}{\partial x_j} \frac{\partial \Pi_0}{\partial p_i} \right],$$
$$\mathcal{H}_2 = -\frac{1}{8} \left[\frac{\partial^2 \Pi_0}{\partial x_i \partial x_j} \frac{\partial^2 \Pi_0}{\partial p_i \partial p_j} - \frac{\partial^2 \Pi_0}{\partial x_i \partial p_j} \frac{\partial^2 \Pi_0}{\partial x_j \partial p_i} \right],$$

and

$$\Pi_0 = \sum_{A=1}^{\mathrm{N}} \lambda_A^{(0)} \widetilde{\mathcal{M}}_A .$$

* * *

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