Quantum hydrodynamic models from a maximum entropy principle

2010 J. Phys. A: Math. Theor. 43 102001

(http://iopscience.iop.org/1751-8121/43/10/102001)

IOP FTC
IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **43** (2010) 102001 (11pp) doi:10.1088/1751-8113/43/10/102001

FAST TRACK COMMUNICATION

Quantum hydrodynamic models from a maximum entropy principle

M Trovato[1] **and L Reggiani**[2]

[1] Dipartimento di Matematica, Università di Catania, Viale A. Doria, 95125 Catania, Italy
[2] Dipartimento di Ingegneria dell' Innovazione and CNISM, Università del Salento, Via Arnesano s/n, 73100 Lecce, Italy

E-mail: trovato@dmi.unict.it

Received 5 December 2009, in final form 24 January 2010
Published 17 February 2010
Online at stacks.iop.org/JPhysA/43/102001

Abstract

We use a density matrix formalism to derive a kinetic theory for a quantum gas. Generalized kinetic fields are introduced and, employing the Wigner function, a certain hierarchy of quantum hydrodynamic (QHD) equations for the corresponding macroscopic variables is obtained. We assert a maximum entropy principle to obtain closure of the QHD system. For the explicit incorporation of statistics a proper quantum entropy is analyzed in terms of the reduced density matrix. The determination of the reduced Wigner function for equilibrium and non-equilibrium conditions is found to become possible only by assuming that the Lagrange multipliers can be expanded in powers of $\hbar^2$. Quantum contributions are expressed in powers of $\hbar^2$ while classical results are recovered in the limit $\hbar \to 0$.

PACS numbers: 67.10.Jn, 89.70.Cf

1. Introduction

A rigorous derivation of a hydrodynamic (HD) model is a fundamental problem in statistical mechanics. The solution stems from the construction of a given number of moments of the particle distribution function. In this derivation, the main difficulty is identified in the closure problem associated with the constraint that to solve a finite set of moment equations the knowledge of higher order moments is necessary [1, 2]. 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]. This is no longer the case in quantum mechanics, apart from some partial attempts [3]. 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, such as interacting fermionic and bosonic gases [4, 5], quantized vortices [6], quantum turbulence [7], confined carrier transport in semiconductor heterostrucures [8], nuclear physics [9].

The aim of this work is to develop a rigorous theoretical approach for constructing a complete set of quantum balance equations and formulate a global quantum maximum entropy principle to solve the corresponding closure problem. To this purpose, the main items of the work will be the following: (i) the definition of the reduced Wigner function for a system of identical particles. (ii) The development of the moments of the reduced Wigner function. (iii) The formulation of the closure problem by a proper definition of a quantum entropy which includes the particle undistinguishable principle. (iv) The introduction and use of quantum Lagrange multipliers to determine the potentials associated with external constraints.

2. The generalized Wigner equation

We consider a given number N of identical particles introducing, 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 general Hamiltonian, with many-body interactions,

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

where, neglecting the spin degree of freedom, Ψ is the particle field operator satisfying the relations $[\Psi(\mathbf{r}), \Psi(\mathbf{r}')]_\pm = [\Psi^\dagger(\mathbf{r}), \Psi^\dagger(\mathbf{r}')]_\pm = 0$, $[\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')]_\pm = \delta(\mathbf{r} - \mathbf{r}')$ and the upper and lower signs refer to fermions and bosons, respectively.

Analogously, in the coordinate space representation we can define the reduced density matrix [10] of a 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 will take the form $\langle \nu|\widehat{\varrho}\,|\nu'\rangle = \langle a^\dagger_{\nu'} a_\nu\rangle = \mathrm{Tr}\left(\rho\, a^\dagger_{\nu'} a_\nu\right)$ being ν, ν' single particle states, $a_\nu, a^\dagger_{\nu'}$ the annihilation and creation operators for these states and $\langle\cdots\rangle$ the statistical mean value. By using this formalism [10], we define the *reduced* Wigner function

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

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 and $n(\mathbf{r})$ is the quasi-particle numerical density, with $\mathrm{Tr}(\widehat{\varrho}) = N$. By looking for a function $\widetilde{\mathcal{M}}(\mathbf{r}, \mathbf{p})$ in phase space that *corresponds* unambiguously to an operator of a single particle $\widehat{\mathcal{M}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$, we introduce the Weyl–Wigner transform $\mathcal{W}(\widehat{\mathcal{M}}) = \widetilde{\mathcal{M}}(\mathbf{r}, \mathbf{p}) = \int \mathrm{d}^3\tau \langle \mathbf{r} + \tau/2|\widehat{\mathcal{M}}|\mathbf{r} - \tau/2\rangle\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tau\cdot\mathbf{p}}$. Analogously, we define the inverse Weyl–Wigner transform $\mathcal{W}^{-1}(\widetilde{\mathcal{M}}) = \langle \mathbf{r}|\widehat{\mathcal{M}}|\mathbf{r}'\rangle = (2\pi\hbar)^{-3} \int \mathrm{d}^3 p\, \widetilde{\mathcal{M}}((\mathbf{r} + \mathbf{r}')/2, \mathbf{p})\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}$. Thus, $\widetilde{\varrho}(\mathbf{r}, \mathbf{p}) = (2\pi\hbar)^3 \mathcal{F}_\mathcal{W}(\mathbf{r}, \mathbf{p})$ 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 [10]

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

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

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

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

where Einstein convention is used on the saturated indices and the effects of interactions are entirely contained in the definition of $V_{\mathrm{eff}}(\mathbf{r})$. We remark that in general the above expansion can be performed only if $V_{\mathrm{eff}}(\mathbf{r})$ is an analytical function in the whole region of interest; thus, the presence of potential discontinuities cannot be treated with this equation. Accordingly, if $V_{\mathrm{eff}}(\mathbf{r})$ does not admit for a Taylor series expansion, then an integro-differential form of the Wigner equation should be used [12, 13]. Finally, for $\hbar \to 0$, we recover a kind of Boltzmann–Liouville equation with an effective potential that includes all interaction effects. The essential difference between classical and the quantum theory is, here, that in the first case, Boltzmann–Liouville equation allows the violation of uncertainty relation in phase space, while in the quantum case the expansion (4) allows us to obtain a non-local theory for the system compatible with the uncertainty principle.

As a relevant application of this approach, we consider a Bose gas with many-body contact interactions [14] 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 $\forall\ k \geqslant 2$ to obtain

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

where $g^{(k)}(\mathbf{r},\ldots,\mathbf{r}) = \langle[\Psi^{\dagger}(\mathbf{r})]^k[\Psi(\mathbf{r})]^k\rangle/[n(\mathbf{r})]^k$ is the k-order correlation function [15]. We stress that, by considering the explicit relation (5), all nonlinear 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 implied by contact interactions are *explicitly determined* as known polynomial functions of the field variable $n(\mathbf{r})$. In this sense a theory based on equations (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 the appendix).

The above results can be formulated by including explicitly the spin degrees of freedom, and equations (3) and (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 [10], non-ideal gases and plasmas [16]. Thus, for a Bose gas, the theory can be generalized introducing the Boltzmann–Nordheim (BN) kinetic equation through the BBGKY hierarchy for the density matrix when the dynamical correlations caused by collisions are supposed to be very well localized both in space and time [17]. In this case, the solution of the coupled equations of the type BN plus equations (4) and (5) should describe, to an higher level of approximation, the dynamics of a Bose–Einstein condensate.

3. QHD models

Below we develop the extended three-dimensional 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 $\langle\widehat{\mathcal{M}}(\widehat{\mathbf{r}},\widehat{\mathbf{p}})\rangle = \iint \mathrm{d}^3p\,\mathrm{d}^3r\,\widetilde{\mathcal{M}}(\mathbf{r},\mathbf{p})\mathcal{F}_{\mathcal{W}}(\mathbf{r},\mathbf{p},t)$, 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 $v_i = n^{-1} \int \mathrm{d}^3 p \; u_i \, \mathcal{F}_{\mathcal{W}}$, 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[3] $\widetilde{\mathcal{M}}_A = \left\{\widetilde{\varepsilon}^s, \widetilde{\varepsilon}^s \widetilde{u}_{i_1}, \ldots, \widetilde{\varepsilon}^s \widetilde{u}_{\langle i_1} \widetilde{u}_{i_2} \cdots \widetilde{u}_{i_r\rangle}\right\}$ 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, by construction, it is $M_{(0)|i_1} = 0$, and

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

with $s = 0, 1, \ldots, \mathcal{N}$ and $r = 1, 2, \ldots, \mathrm{M}$. 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 $s = 0, \ldots, \mathcal{N}$. 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 $M_{(1)} = 3/2P$ 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 also consider some scalar and vectorial moments of higher order. Multiplying (4) by $\widetilde{\mathcal{M}}_A$, integrating over $\mathbf{p}$ we exactly determine the corresponding set of quantum balance equations to all orders of $\hbar$. 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 the balance equations can be expressed explicitly as

$$\dot{n} + n \, \frac{\partial v_k}{\partial x_k} = 0, \tag{7}$$

$$\dot{v}_i + \frac{1}{n} \, \frac{\partial M_{(0)|ik}}{\partial x_k} + \frac{1}{m} \, \frac{\partial V_{\mathrm{eff}}}{\partial x_i} = 0, \tag{8}$$

$$\begin{aligned} \dot{M}_{(s)} + M_{(s)} \, \frac{\partial v_k}{\partial x_k} + \frac{\partial M_{(s)|k}}{\partial x_k} + s\, m \, M_{(s-1)|ik} \, \frac{\partial v_i}{\partial x_k} - s \frac{m}{n} \, M_{(s-1)|i} \, \frac{\partial M_{(0)|ik}}{\partial x_k} = \frac{\hbar^2}{24} \, s(s-1) \\ \times \left\{ (s-2) \, \frac{\partial^3 V_{\mathrm{eff}}}{\partial x_{\langle i} \partial x_j \partial x_{k\rangle}} \, M_{(s-3)|\langle ijk\rangle} + \frac{3}{5} \frac{(1+2s)}{m} \, \frac{\partial^3 V_{\mathrm{eff}}}{\partial x_r \partial x_r \partial x_k} \, M_{(s-2)|k} \right\}, \end{aligned} \tag{9}$$

$$\begin{aligned} \dot{M}_{(s)|i} + M_{(s)|i} \, \frac{\partial v_k}{\partial x_k} + \frac{\partial M_{(s)|ik}}{\partial x_k} + sm M_{(s-1)|ijk} \, \frac{\partial v_j}{\partial x_k} + M_{(s)|k} \, \frac{\partial v_i}{\partial x_k} - \frac{M_{(s)}}{n} \, \frac{\partial M_{(0)|ik}}{\partial x_k} \\ - sm \, \frac{M_{(s-1)|ij}}{n} \, \frac{\partial M_{(0)|jk}}{\partial x_k} = \frac{\hbar^2}{24} \, s \left\{ (s-1)(s-2) \, \frac{\partial^3 V_{\mathrm{eff}}}{\partial x_r \partial x_j \partial x_k} \, M_{(s-3)|\langle rjki\rangle} \right. \\ + \frac{3(s-1)}{m} \, \frac{(3+2s)}{7} \left(\frac{\partial^3 V_{\mathrm{eff}}}{\partial x_r \partial x_r \partial x_k} \, M_{(s-2)|\langle ki\rangle} + \frac{\partial^3 V_{\mathrm{eff}}}{\partial x_{\langle k} \partial x_{r\rangle} \partial x_i} \, M_{(s-2)|\langle kr\rangle} \right) \\ \left. + \frac{(4s^2 + 8s + 3)}{5\, m^2} \, \frac{\partial^3 V_{\mathrm{eff}}}{\partial x_r \partial x_r \partial x_i} \, M_{(s-1)} \right\} \qquad \text{with} \quad s = 1, \ldots, \mathcal{N}. \end{aligned} \tag{10}$$

We remark that, by considering the complete expansion (4), it follows that only a finite number of terms in powers of $\hbar^2$ remains in each QHD scalar and vectorial equation, and the first quantum correction, on the right-hand side, involves the third derivative of V_{eff}. The set (7)–(10) is a second major result of the work and, for $\hbar \to 0$, it recovers the classic form of extended thermodynamics [1, 18]. However, for assigned expressions of V_{eff},

[3] $A_{\langle i_1 \cdots i_n\rangle}$ is the traceless symmetric part of tensor $A_{i_1 \cdots i_n}$.

the predictive power and convergence properties of this system should be investigated via numerical calculations.

The previous set of equations contains unknown constitutive functions which, through (6), are represented by the central moments of higher order $H_A = \{M_{\mathcal{N}+1},\ M_{(s)|\langle ij\rangle},\ M_{(l)|\langle ijk\rangle},\ M_{(p)|\langle ijqk\rangle}\}$ with $s = 0,\ldots,\mathcal{N}$; $l = 0,\ldots,\mathcal{N}-1$ and $p = 0,\ldots,\mathcal{N}-3$.

In general, the closure problem of a set of balance equations is tackled using the QMEP formalism [3].

4. The QMEP approach

In order to take into account *ab initio* the Bose and Fermi statistics, we follow the Landau strategy [19]. Thus, for a non-interacting system in non-equilibrium conditions, the quantum entropy, for the whole system, can be determined in terms of the occupation numbers in the form $S = -k_B \sum_\nu y[\langle\overline{N_\nu}\rangle \ln\langle\overline{N_\nu}\rangle \pm (1 \mp \langle\overline{N_\nu}\rangle)\ln(1 \mp \langle\overline{N_\nu}\rangle)]$ where k_B is the Boltzmann constant, $\langle\overline{N_\nu}\rangle = \langle a_\nu^\dagger a_\nu\rangle/y$, $y = (2\tilde{s}+1)$, is the spin degeneration and the upper and lower signs refer to fermions and bosons, respectively. If we consider the Schrodinger equation of a single particle $[\widehat{\mathcal{H}}(\mathbf{r}) - E_\nu]\varphi_\nu(\mathbf{r}) = 0$, then, in stationary conditions, both the reduced density matrix $\widehat{\varrho}$ and any operator $\widehat{\Phi}(\widehat{\varrho})$ are diagonal in the base φ_ν. Thus, introducing as a function of reduced density matrix $\widehat{\varrho}$ the following quantity:

$$\widehat{\Phi}(\widehat{\varrho}) = \widehat{\varrho}\left\{\ln\left(\frac{\widehat{\varrho}}{y}\right) \pm y\,\hat{\varrho}^{-1}\left(\widehat{I} \mp \frac{\widehat{\varrho}}{y}\right)\ln\left(\widehat{I} \mp \frac{\widehat{\varrho}}{y}\right)\right\}, \tag{11}$$

with $\widehat{I}$ the identity, we have $\langle\nu|\widehat{\varrho}\,|\nu'\rangle = \langle a_\nu^\dagger a_\nu\rangle\delta_{\nu\nu'}$ and $\langle\nu|\widehat{\Phi}(\widehat{\varrho})|\nu'\rangle = y[\langle\overline{N_\nu}\rangle\ln\langle\overline{N_\nu}\rangle \pm(1 \mp \langle\overline{N_\nu}\rangle)\ \ln(1 \mp \langle\overline{N_\nu}\rangle)]\delta_{\nu\nu'}$. Consequently, by generalizing existing definitions [20], the Bose or Fermi statistics can be implicitly taken into account by defining the quantum entropy, for the whole system, in terms of the functional of the reduced density matrix

$$S(\widehat{\varrho}) = -k_B\,\mathrm{Tr}(\widehat{\Phi}(\widehat{\varrho})), \tag{12}$$

where k_B is the Botzmann constant and $\widehat{\Phi}(\widehat{\varrho})$ is given by (11). To explain the QMEP approach in the space of phase, we introduce the corresponding phase function $\widetilde{\Phi}(\mathbf{r},\mathbf{p}) = \mathcal{W}(\widehat{\Phi})$, rewriting (12) as $S(\widehat{\varrho}) = -k_B\,(2\pi\hbar)^{-3}\iint \mathrm{d}^3p\,\mathrm{d}^3r\,\mathcal{W}(\widehat{\Phi})$, and we search the extremal value of entropy subject to the constraint that the information on the physical system is described by $M_A(\mathbf{r},t)$. To this purpose, we consider the new *global* functional [3]

$$\widetilde{S} = S - \int \mathrm{d}^3r\left\{\sum_{A=1}^{\mathrm{N}}\widetilde{\lambda}_A\left[\int \mathrm{d}^3p\,\widetilde{\mathcal{M}}_A\,\mathcal{F}_\mathcal{W} - M_A\right]\right\} \tag{13}$$

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

$$\widehat{\varrho} = y\left\{\exp\left[\mathcal{W}^{-1}\left(\sum_{A=1}^{\mathrm{N}}\lambda_A(\mathbf{r},t)\,\widetilde{\mathcal{M}}_A\right)\right] \pm \widehat{I}\right\}^{-1} \tag{14}$$

with $\lambda_A = \widetilde{\lambda}_A/k_B$. Equation (14) is a third major result of the work, and the reduced Wigner function takes the form

$$\mathcal{F}_\mathcal{W} = \frac{1}{(2\pi\hbar)^3}\,\mathcal{W}(\widehat{\varrho}[\lambda_A(\mathbf{r},\,t),\,\widetilde{\mathcal{M}}_A]). \tag{15}$$

We stress that, to take into account the detailed kinetics of the interactions, we consider the above approach in a dynamical context. Indeed, 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. Thus, from the knowledge of the functional form (14) and (15) of the reduced Wigner function, we use (4) to obtain a set of equations for the constraints. This set completely represents the closed QHD_2 model (7)–(10) 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 correction terms. In particular, by using the Moyal formalism, one can prove [12, 13, 21] that the Wigner function, and hence the central moments, can be expanded in even power of $\hbar$:

$$\mathcal{F}_{\mathcal{W}} = \sum_{k=0}^{\infty} \hbar^{2k} \mathcal{F}_{\mathcal{W}}^{(2k)}, \qquad M_A = \sum_{k=0}^{\infty} \hbar^{2k} M_A^{(2k)}. \tag{16}$$

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

$$M_A = \frac{1}{(2\pi\hbar)^3} \int \mathrm{d}^3 p \, \widetilde{\mathcal{M}}_A \, \mathcal{W}(\widehat{\varrho}[\lambda_B(\mathbf{r}, t), \widetilde{\mathcal{M}}_B]). \tag{17}$$

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

$$\lambda_A = \lambda_A^{(0)} + \sum_{k=1}^{\infty} \hbar^{2k} \lambda_A^{(2k)}. \tag{18}$$

With these assumptions, and using (14) and (15), we succeed in determining the following expression for $\mathcal{F}_W$:

$$\mathcal{F}_{\mathcal{W}} = \frac{\widetilde{y}}{\mathrm{e}^{\Pi} \pm 1} \left\{ 1 + \sum_{r=1}^{\infty} \hbar^{2r} P_{2r}^{\pm} \right\}, \tag{19}$$

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

(19) 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 (17). In this case, M_A must satisfy the QHD_2 system (7)–(10). From the knowledge of the Lagrange multipliers, both the Wigner function and the constitutive functions H_A can be determined explicitly.

5. Some examples of the QMEP approach

By considering only the first two terms of (19), we decompose the Lagrange multipliers in the local equilibrium and non-equilibrium parts, $\Pi = \alpha + \beta\, \tilde{\varepsilon} + \sum \Lambda_A \widetilde{\mathcal{M}}_A$, $\{\alpha(\mathbf{r}, t),\ \beta(\mathbf{r}, t)\}$ being the non-vanishing Lagrange multipliers of local equilibrium, and $\Lambda_A(\mathbf{r}, t)$ the non-equilibrium Lagrange multipliers. Thus, by taking an expansion up to the first order with respect to the deviations from the local equilibrium configuration $\mathcal{F}_{\mathcal{W}}|_E$, we obtain a theory limited to states

near local equilibrium, being

$$\mathcal{F}_{\mathcal{W}}|_E = \widetilde{y}\left[L^{\pm}_{(0)} + \hbar^2 P_2^{\pm(0)}\right]$$

$$\mathcal{F}_{\mathcal{W}}|_{NE} = \widetilde{y}\left[L^{\pm}_{(1)} + \hbar^2 P_2^{\pm(1)}\right] \sum_{l=0}^{N} \left\{\Lambda_{(l)}\tilde{\varepsilon}^l + \Lambda_{(l)|i}\tilde{\varepsilon}^l\tilde{u}_i\right\},$$

where the functions $L^{\pm}_{(n)}$ are given by

$$L^{\pm}_{(s)} = \frac{d^s}{d\alpha^s}\left\{\frac{1}{\mathrm{e}^{\alpha+\beta\tilde{\varepsilon}} \pm 1}\right\}.$$

For the sake of simplicity we assume that non-local effects are imputable only to the spatial derivatives of density n; thus, the quantum correction terms $P_2^{\pm(r)}$ (with $r = 0, 1$) are expressed in the form

$$P_2^{\pm(r)} = \frac{1}{12m}\frac{1}{k_B T}\left\{\left[L^{\pm}_{(3+r)}Q^{(1)} + 9L^{\pm}_{(2+r)}Q^{(2)}\right] + \frac{m}{k_B T}L^{\pm}_{(3+r)}\left[Q^{(2)}\tilde{u}^2 + Q_{\langle ij\rangle}\tilde{u}_{\langle i}\tilde{u}_{j\rangle}\right]\right\} + \mathcal{O}(\hbar^2),$$

where T is an effective temperature and the non-local quantities $\{Q^{(k)},\ Q_{\langle ij\rangle}\}$ are explicitly reported in the appendix. With this approach we can invert, order by order, the constrains (17) determining explicitly the Lagrange multipliers and consequently the closure relations for the system (7)–(10). Thus, for example, by considering the QHD$_2$ obtained for $\mathcal{N} = 0, 1$ we determine the following closed systems.

For $\mathcal{N} = 0$, we recover the usual quantum drift-diffusion model with the balance equations (7) and (8) for the macroscopic variables $\{n,\ v_i\}$, $M_{(0)|ik} = M_{(0)|\langle ik\rangle} + P/m\,\delta_{ik}$ being the unknown constitutive function. In this case the effective temperature $T = T_0$ is necessarily constant (with $\beta = (k_B T_0)^{-1}$), the pressure P and the traceless tensor $M_{(0)|\langle ik\rangle}$ being determined by relations

$$P = \frac{2}{3}n\frac{I^{\pm}_4}{I^{\pm}_2}\left\{k_B T_0 + \frac{\hbar^2}{8m}\left[\frac{1}{4}\left(\frac{I^{\pm}_{-2}}{I^{\pm}_4} + \frac{I^{\pm}_{-4}}{I^{\pm}_2}\right)Q^{(1)} + \left(2\frac{I^{\pm}_0}{I^{\pm}_4} + \frac{I^{\pm}_{-2}}{I^{\pm}_2}\right)Q^{(2)}\right]\right\} + \mathcal{O}(\hbar^4) \tag{20}$$

$$M_{(0)|\langle ik\rangle} = -\frac{\hbar^2}{12}\frac{n}{m^2}\frac{I^{\pm}_0}{I^{\pm}_2}Q_{\langle ik\rangle} + \mathcal{O}(\hbar^4), \tag{21}$$

where, in general, all statistics information is contained, for any value of α, in the Fermi and Bose integral functions $I^{\pm}_n(\alpha)$ (see the appendix) while the non-locality is expressed by terms $\{Q^{(k)},\ Q_{\langle ij\rangle}\}$. We remark that, for $\alpha \gg 1$, as a particular case, we obtain the well-known results determined in the framework of the Boltzmann statistic for the quantum drift-diffusion model. Thus, we have $I^{\pm}_n(\alpha) \approx (1/2)\,\Gamma\,[(n+1)/2]\,\exp(-\alpha)$ and we obtain

$$M_{(0)|ik} = \frac{n}{m}\left\{k_B T_0\delta_{ik} - \frac{\hbar^2}{12m}\frac{\partial^2 \ln n}{\partial x_i \partial x_k}\right\} + \mathcal{O}(\hbar^4).$$

It is easy to verify that, by introducing the usual Bohm quantum potential $Q_B = -(\hbar^2/2m\sqrt{n})\,\triangle\sqrt{n}$, we recover the known closure relation, for nondegenerate gases, [22]

$$\frac{\partial M_{(0)|ik}}{\partial x_k} = \frac{k_B T_0}{m}\frac{\partial n}{\partial x_i} + \frac{n}{3m}\frac{\partial Q_B}{\partial x_i} + \mathcal{O}(\hbar^4).$$

For $\mathcal{N} = 1$, we consider the QHD$_2$ system (7)–(10) for the macroscopic variables $\{n,\ v_i,\ P,\ q_i\}$, which admits for a direct physical interpretation, the *pressure* being $P = 2/3\,M_{(1)}$ and the *heat flux density* $q_i = M_{(1)|i}$. Accordingly, we find the balance equations

$$\frac{\partial n}{\partial t} + \frac{\partial n\, v_k}{\partial x_k} = 0, \tag{22}$$

$$\frac{\partial v_i}{\partial t} + v_k \frac{\partial v_i}{\partial x_k} + \frac{1}{n}\frac{\partial}{\partial x_k}\left\{M_{(0)|\langle ik\rangle} + \frac{P}{m}\delta_{ik}\right\} + \frac{1}{m}\frac{\partial V_{\rm eff}}{\partial x_i} = 0, \tag{23}$$

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial x_k}\left\{P\, v_k + \frac{2}{3} q_k\right\} + \frac{2}{3} P \frac{\partial v_k}{\partial x_k} + \frac{2}{3} m\, M_{(0)|\langle ik\rangle}\frac{\partial v_i}{\partial x_k} = 0, \tag{24}$$

$$\begin{aligned}\frac{\partial q_i}{\partial t} + \frac{\partial}{\partial x_k}\left\{q_i\, v_k + M_{(1)|\langle ik\rangle} + \frac{2}{3}\frac{1}{m} M_{(2)}\,\delta_{ik}\right\} + m\, M_{(0)|\langle ijk\rangle}\frac{\partial v_j}{\partial x_k} - \frac{5}{2}\frac{P}{n}\frac{\partial}{\partial x_k} \\ \times\left\{M_{(0)|\langle ik\rangle} + \frac{P}{m}\delta_{ik}\right\} - \frac{m}{n} M_{(0)|\langle ij\rangle}\frac{\partial}{\partial x_k}\left\{M_{(0)|\langle jk\rangle} + \frac{P}{m}\delta_{jk}\right\} \\ + \frac{2}{5} q_i \frac{\partial v_k}{\partial x_k} + \frac{2}{5} q_k \frac{\partial v_k}{\partial x_i} + \frac{7}{5} q_k \frac{\partial v_i}{\partial x_k} = \frac{\hbar^2}{8m^2} n \frac{\partial^3 V_{\rm eff}}{\partial x_k \partial x_k \partial x_i}.\end{aligned} \tag{25}$$

In this case, the effective temperature is expressed by means of the equation $k_B\, T = (3\, P/2\, n)\left(I_2^{\pm}/I_4^{\pm}\right)$, and the constitutive functions $H_A = \{M_{(0)|\langle ik\rangle}, M_{(1)|\langle ik\rangle}, M_{(0)|\langle ijk\rangle}, M_{(2)}\}$ will be given through the general relations

$$M_{(0)|\langle ik\rangle} = -\frac{1}{12}\frac{\hbar^2}{m^2} n \frac{I_0^{\pm}}{I_2^{\pm}} Q_{\langle ik\rangle} + \mathcal{O}(\hbar^4), \tag{26}$$

$$M_{(1)|\langle ik\rangle} = -\frac{7}{12}\frac{\hbar^2}{m^2} n\, k_B\, T\; Q_{\langle ik\rangle} + \mathcal{O}(\hbar^4), \tag{27}$$

$$M_{(0)|\langle ijk\rangle} = \frac{3}{4}\frac{\hbar^2}{m^2}\frac{\Phi}{k_B\, T}\; q_{\langle i}\, Q_{\langle jk\rangle\rangle} + \mathcal{O}(\hbar^4), \tag{28}$$

$$M_{(2)} = n\, \frac{I_6^{\pm}}{I_2^{\pm}}\, (k_B\, T)^2 \left\{1 + \frac{\hbar^2}{12\, m}\frac{1}{k_B\, T}\left[\zeta_1\, Q^{(1)} + \zeta_2\, Q^{(2)}\right]\right\} + \mathcal{O}(\hbar^4), \tag{29}$$

where the coefficients $\{\Phi,\ \zeta_1,\ \zeta_2\}$ are given in the appendix. We remark that the closure relations (26)–(29) are valid for arbitrary values of α being expressed in terms of Fermi and Bose integral functions. Also in this case, for $\alpha \gg 1$ we obtain, in the framework of Boltzmann statistic, $P = n\, k_B\, T$ and the following simplified non-local closure relations for nondegenerate gases:

$$\begin{aligned} M_{(0)|\langle ik\rangle} &= -\frac{1}{12}\frac{\hbar^2}{m^2} n \frac{\partial^2 \ln n}{\partial x_{\langle i}\partial x_{k\rangle}} + \mathcal{O}(\hbar^4) \\ M_{(1)|\langle ik\rangle} &= -\frac{7}{24}\frac{\hbar^2}{m^2} n k_B T \frac{\partial^2 \ln n}{\partial x_{\langle i}\partial x_{k\rangle}} + \mathcal{O}(\hbar^4) \\ M_{(0)|\langle ijk\rangle} &= -\frac{1}{5}\frac{\hbar^2}{m^2}\frac{1}{k_B T} q_{\langle i}\frac{\partial^2 \ln n}{\partial x_{\langle j}\partial x_{k\rangle\rangle}} + \mathcal{O}(\hbar^4) \\ M_{(2)} &= \frac{15}{4} n\, (k_B T)^2 + \mathcal{O}(\hbar^4). \end{aligned}$$

6. Conclusion

The QMEP is here proposed as a rigorous, non-arbitrary procedure that can be employed when it becomes necessary to treat systems in partially specified quantum mechanical states. In this

respect we have shown that (a) by introducing the generalized quantum entropy (11) and (12), we incorporate the quantum statistics into problems involving a system of identical particles. (b) By using the Wigner representation we formulate a QMEP, which requires the consistent introduction of quantum Lagrange multipliers, to obtain a non-local theory for the system. (c) We determine a closed QHD for the macroscopic variables used as constraints in the QMEP approach. (d) In the limit $\hbar \to 0$, we recover $\lambda_A^{(0)} = \lambda_A^{(0)}\big(M_B^{(0)}\big)$ and $\mathcal{F}_{\mathcal{W}}^{(0)}$ obtained in the classic MEP approach [1] for a fermions or bosons system.

Acknowledgments

This work is dedicated to the memory of Professor A M Anile. The communication is supported by INDAM-GNFM project *Young Researchers* (2008), MIUR-PRIN project *Nonlinear Propagation and Stability in Thermodynamical Processes of Continuous Media* and MADESS II project of the Italian National Research Council (CNR).

Appendix A.

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

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

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

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

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

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

By inserting the term $\partial\varphi/\partial t|_L$ in (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 (A.3) in (A.2), we obtain the term which describes the nonlinear dynamics:

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

where $\varphi^*(\mathbf{r}-\tau/2,\,t)\,\varphi(\mathbf{r}+\tau/2,\,t) = \int \mathrm{d}^3p'\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\tau\cdot\mathbf{p}'}\mathcal{F}_{\mathcal{W}}$ and $F_j(\mathbf{r}\pm\tau/2,t) = |\varphi(\mathbf{r}\pm\tau/2,t)|^{2j}$. By expanding the quantities $F_j(\mathbf{r}\pm\tau/2,t)$ in series around $\tau = 0$, and assuming that all

derivatives of $\mathcal{F}_{\mathcal{W}}$ vanish when $\mathbf{r}, \mathbf{p} \to \infty$, we find

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

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

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

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

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

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

We remark that for $R = 2$ (Gross–Pitaevskii equation) relation (A.6) coincides exactly with (5). Analogously, by considering (5) for $R > 2$, a reasonable description of the low-energy dynamics can be given assuming values approximatively constant for the remaining correlation functions (see section 7.6, in [15]). Thus, also in this case (A.6) can be determined as a particular case of (5).

Closure relations. We define the Fermi and the Bose integral functions for $s \geqslant 0$:

$$I_s^{\pm}(\alpha) = \int_0^{+\infty} \frac{x^s}{\exp(\alpha + x^2) \pm 1}\, \mathrm{d}x$$

satisfying the differentiation property

$$\frac{\mathrm{d}^r I_s^{\pm}(\alpha)}{\mathrm{d}\alpha^r} = (-1)^r \frac{\Gamma\left(\frac{s+1}{2}\right)}{\Gamma\left(\frac{s+1}{2} - r\right)} I_{s-2r}^{\pm}(\alpha)$$

that is also used to extend the definition of $I_s^{\pm}(\alpha)$ to $s < 0$.

The non-local terms $\{Q^{(1)},\ Q^{(2)},\ Q_{\langle ij\rangle}\}$ are expressed by

$$Q^{(1)} = -2\left(\frac{I_2^{\pm}}{I_0^{\pm}}\right)^2 \left(\frac{\partial \ln n}{\partial x_k}\right)^2,$$

$$Q^{(2)} = \frac{1}{3}\frac{I_2^{\pm}}{I_0^{\pm}} \left\{ \left[1 + \frac{I_2^{\pm}}{I_0^{\pm}} \frac{I_{-2}^{\pm}}{I_0^{\pm}} \right] \left(\frac{\partial \ln n}{\partial x_k}\right)^2 + \frac{\partial^2 \ln n}{\partial x_k \partial x_k} \right\}$$

$$Q_{\langle ij\rangle} = \frac{I_2^{\pm}}{I_0^{\pm}} \left\{ \left[1 + \frac{I_2^{\pm}}{I_0^{\pm}} \frac{I_{-2}^{\pm}}{I_0^{\pm}} \right] \frac{\partial \ln n}{\partial x_{\langle i}} \frac{\partial \ln n}{\partial x_{j\rangle}} + \frac{\partial^2 \ln n}{\partial x_{\langle i} \partial x_{j\rangle}} \right\}$$

Accordingly, the coefficients $\{\Phi,\ \zeta_1,\ \zeta_2\}$, contained in the constitutive functions (28) and (29), are given by relations

$$\Phi = \frac{27\left(I_2^{\pm}\right)^2 - 5 I_0^{\pm} I_4^{\pm}}{25\left(I_4^{\pm}\right)^2 - 21 I_2^{\pm} I_6^{\pm}}, \qquad \zeta_1 = -\frac{3}{8}\left[\frac{I_{-4}^{\pm}}{I_2^{\pm}} + 2\frac{I_{-2}^{\pm}}{I_4^{\pm}} + 5\frac{I_0^{\pm}}{I_6^{\pm}} \right]$$

$$\zeta_2 = -\frac{3}{2}\left[\frac{I_{-2}^{\pm}}{I_2^{\pm}} + 4\frac{I_0^{\pm}}{I_4^{\pm}} - 5\frac{I_2^{\pm}}{I_6^{\pm}} \right].$$

References

[1] Müller I and Ruggeri T 1998 *Rational Extended Thermodynamics*, Springer Tracts in Natural Philosophy Vol 37 (New York: Springer-Verlag)
[2] Trovato M and Reggiani L 2006 *Phys. Rev.* B **73** 245209 and references therein
[3] Jaynes E T 1957 *Phys. Rev.* **108** 171
Degond P and Ringhofer C 2003 *J. Stat. Phys.* **112** 587
[4] Chamon C, Oshikawa M and Affleck I 2003 *Phys. Rev. Lett.* **20** 206403
[5] Bulgac A 2002 *Phys. Rev. Lett.* **89** 050402
[6] Eltsov V B, Finne A P, Hanninen R, Kopu J, Krusius M, Tsubota M and Thuneberg E V 2006 *Phys. Rev. Lett.* **96** 215302
[7] Kobayashi M and Tsubota M 2005 *Phys. Rev. Lett.* **94** 65302
[8] Frensley W 1990 *Rev. Mod. Phys.* **62** 745
[9] Kartavenko V G 1984 *Sov. J. Nucl. Phys.* **40** 240
[10] Klimontovich Yu 1958 *Soviet Phys. JETP* **6** 753
Silin V P 1958 *Soviet Phys. JETP* **6** 387
Brittin W E and Chappell W R 1962 *Rev. Mod. Phys.* **34** 620
Yang C N 1962 *Rev. Mod. Phys.* **34** 694
[11] Ploszajczak M and Rhoades-Brown M J 1985 *Phys. Rev. Lett.* **55** 147
Ploszajczak M and Rhoades-Brown M J 1986 *Phys. Rev.* D **33** 333686
[12] Wigner E P 1932 *Phys. Rev.* **40** 749
[13] Hillery M, O'Conell R, Scully M and Wigner E P 1984 *Phys. Rep.* **106** 121
[14] Fersino E, Mussardo G and Trombettoni A 2008 *Phys. Rev.* A **7** 053608
[15] Parkins A S and Walls D F 1998 *Phys. Reports* **303** 71 and references therein
[16] Klimontovich Yu 1982 *Kinetic theory of nonideal gases & nonideal plasmas*, International series in Natural Philosophy Vol 105 (Oxford: Pergamon) and references therein
[17] Escobedo M and Velázquez J J L 2008 *J. Phys. A: Math. Theor.* **41** 395208
[18] Reinecke S and Kremer G M 1990 *Phys. Rev.* A **42** 815
[19] Landau L D and Lifshitz E M 1959 *Statistical Physics* (Course of Theoretical Physics) Vol 5 (London-Paris: Pergamon Press) p 154
[20] Wehrl A 1978 *Rev. Mod. Phys.* **50** 221
Manfredi G and Feix M R 2000 *Phys. Rev.* E **62** 4665
[21] Carruthers P and Zachariasen F 1983 *Rev. Mod. Phys.* **55** 245
[22] Gardner C and Ringhofer C 1996 *Phys. Rev.* E **53** 157