

Quantum maximum-entropy principle for closed quantum hydrodynamic transport within a Wigner function formalism

M. Trovato¹ and L. Reggiani²¹*Dipartimento di Matematica, Università di Catania, Viale A. Doria, I-95125 Catania, Italy*²*Dipartimento di Ingegneria dell' Innovazione and CNISM, Università del Salento, Via Arnesano s/n, I-73100 Lecce, Italy*

(Received 23 February 2011; revised manuscript received 30 September 2011; published 27 December 2011)

By introducing a quantum entropy functional of the reduced density matrix, the principle of quantum maximum entropy is asserted as *fundamental principle of quantum statistical mechanics*. Accordingly, we develop a comprehensive theoretical formalism to construct rigorously a closed quantum hydrodynamic transport within a Wigner function approach. The theoretical formalism is formulated in both thermodynamic equilibrium and nonequilibrium conditions, and the quantum contributions are obtained by only assuming that the Lagrange multipliers can be expanded in powers of \hbar^2 . In particular, by using an arbitrary number of moments, we prove that (1) on a macroscopic scale all nonlocal effects, compatible with the uncertainty principle, are imputable to high-order spatial derivatives, both of the numerical density n and of the effective temperature T ; (2) the results available from the literature in the framework of both a quantum Boltzmann gas and a degenerate quantum Fermi gas are recovered as a particular case; (3) the statistics for the quantum Fermi and Bose gases at different levels of degeneracy are explicitly incorporated; (4) a set of relevant applications admitting exact analytical equations are explicitly given and discussed; (5) the quantum maximum entropy principle keeps full validity in the classical limit, when $\hbar \rightarrow 0$.

DOI: [10.1103/PhysRevE.84.061147](https://doi.org/10.1103/PhysRevE.84.061147)

PACS number(s): 05.60.Gg, 72.20.Ht, 52.25.Kn

I. INTRODUCTION

Hydrodynamical (HD) models consist of a coupled set of partial differential equations for the relevant physical variables of a particle ensemble and are essential for a physical-mathematical description of the space-time evolution of any kind of fluid. A rigorous derivation of an HD model stems from the construction of a given number of moments of the particle distribution function defined in phase space. In this derivation, the main difficulty is identified in the closure problem associated with the constraint that to solve a set of N moment equations it is necessary the knowledge of higher-order moments [1–6]. In classical mechanics, the theory of extended thermodynamics [1,7,8] is a very fruitful approach to study nonequilibrium phenomena using the HD moment equations. This theory provides a systematic method to obtain the constitutive relations present in the hierarchy of moments by using, to any degree of approximation, the maximum entropy principle (MEP) [1,2,7]. Apart from some partial attempts [9–11] this is no longer the case in quantum mechanics. Here the main difficulties are concerned with (1) the definition of a proper quantum entropy that includes particle indistinguishability and (2) the formulation of a global quantum MEP (QMEP) that allows one to obtain a quantum distribution function both for thermodynamic equilibrium and nonequilibrium configurations. Furthermore, in the framework of a nonlocal quantum theory, the generalization of the corresponding Lagrange multipliers is also an open problem. On the other hand, the rigorous formulation of quantum HD (QHD) closed models is a demanding issue for many kinds of problems in quantum systems, like interacting fermionic and bosonic gases [12], quantum turbulence [13], quantum fluids [14], quantized vortices [15], nuclear physics [16], confined carrier transport in semiconductor heterostructures [17], phonon and electron transport in nanostructures [18,19], and nanowires and thin layers [20–22].

Recently, in a series of two papers [5,6] we have presented a set of results addressing this problem by emphasizing the role played by a proper definition of a quantum entropy principle to close quantum hydrodynamic models. Here, by further elaborating previous findings, we provide a comprehensive theoretical formulation of quantum hydrodynamic transport by reporting in explicit form the QHD equations for the cases of a Fermi and Bose gas at different levels of degeneracy. Accordingly, the main objective of the paper is to give an advanced theoretical framework on the application of the maximum entropy principle in quantum statistics. A novel aspect of the present paper concerns the treatment of nonlocal effects, which are here captured not only in terms of spatial derivatives of the density, as already suggested in Ref. [6], but also in terms of spatial derivatives of the temperature.

Starting from the derivation of a generalized Wigner equation, we construct a complete set of quantum balance equations and develop a global QMEP to solve the corresponding closure problem. In this way, within the framework of nonequilibrium Wigner theory, we generalize all the results known in literature both in terms of the statistical effects and in terms of a nonlocal description. Then, on a macroscopic scale, we prove that all nonlocal effects of quantum mechanics on a quantum gas are due to high-order spatial derivatives, both of the numerical density n and of an effective temperature T . In particular, if all the terms associated with the temperature gradient are negligible with respect to the terms connected with the density gradient (DG), then we reobtain all the well-known results determined for a quantum Boltzmann gas [23,24], for a completely degenerate Fermi gas [25–27], and, more generally, some recent results [6] concerning Fermi and/or Bose gases for any level of degeneracy. We remark that, in the case of isothermal conditions (or analogously, for small spatial variations of the temperature), the DG method captures many of the important quantum effects, as confinement and tunneling quantum processes, for physical

systems in the deca-nanometer regime, by offering an approach complementary to existing kinetic methods [18,19]. However, the recent literature has reported on some physical systems in which the mean-free path of the particles is long compared with the scale length of temperature gradients, and hence other nonlocal phenomena should be considered. In these cases, different theoretical models [20] of energy transport have been actively explored, introducing (as new thermodynamic forces) nonlinear products of the temperature gradient, to describe heat transport properties in (1) nanoscale electronic devices, (2) nanowires, (3) thin layers materials, (4) plasma physics, etc. In particular, experiments and simulations of heat transport along these devices have showed results that differ significantly from those predicted by the classic Fourier law [21]. Indeed, on a small scale length even a small difference in temperature can generate very high gradients, whose nonlocal effects cannot be neglected [21,22]. In the framework of Wigner formalism, the QMEP procedure incorporates in a natural way these temperature gradient corrections that, in turn, are of great relevance for the analysis of engineering-oriented devices under quantum nanometer regimes. Finally, we stress that, within the present approach, a proper nonlocal formulation of QMEP is developed in both thermodynamic equilibrium and nonequilibrium conditions. As a consequence, all Lagrange multipliers and the constitutive relations have been explicitly determined in terms of quantum corrections that take into account the nonlocal effects in both equilibrium and nonequilibrium conditions.

To achieve the above objectives, the work is organized as follows. In Sec. II, within a second-quantized formalism, we introduce the reduced density matrix of a single particle and develop the corresponding Wigner dynamics. Section III constructs the extended hydrodynamic system of equations associated with the appropriate Wigner function. In Sec. IV we assert a maximum entropy principle, and, to explicitly incorporate particle indistinguishability, a proper global quantum entropy is analyzed in terms of the reduced density matrix. Section V reports the Moyal expansion of the Wigner function. By using an arbitrary number of scalar and vectorial moments, the expansion of the Wigner function around local equilibrium is investigated in Sec. VI. Sections VII and VIII report the determination of the Lagrange multipliers and the closure relations for different quantum regimes of Fermi and Bose gases, respectively. The case of the first three quantum hydrodynamic systems obtained for a limited set of scalar and vectorial moments of the distribution is illustrated explicitly in Sec. IX. Major conclusions are drawn in Sec. X.

The derivation of analytical results is summarized in an Appendix where we collect mathematical details for the exact determination of (1) the QHD system to all orders of \hbar , (2) the Wigner transform for the QMEP reduced density operator, and (3) the nonlocal expansion, in differential form, both for the Lagrange multipliers and for the closure relations. Throughout this paper the tensor index notation is used; thus for a generic tensor A of rank n , $A_{i_1\dots i_n}$ denotes its components, $A_{(i_1\dots i_n)}$ the symmetric part, and $A_{\langle i_1\dots i_n \rangle}$ the traceless symmetric part. Overall, there are $(2n + 1)$ independent components and the following constraints:

$$A_{(i_1\dots k\dots l\dots i_n)} = A_{(i_1\dots l\dots k\dots i_n)}, \quad A_{\langle i_1\dots k\dots k\dots i_n \rangle} = 0.$$

II. THE WIGNER DYNAMICS

Following Refs. [5,6] we consider a fixed number N of identical particles, and we introduce in Fock space the statistical density matrix ρ for the whole system, with $\text{Tr}(\rho) = 1$ (we suppress the symbol $\hat{}$ to refer to operators acting in Fock space) and the general Hamiltonian

$$H = \int d^3r \Psi^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \Psi(\mathbf{r}) + \sum_{k=2}^L \frac{1}{k!} \int d^3r_1 \cdots \int d^3r_k \Psi^\dagger(\mathbf{r}_1) \cdots \Psi^\dagger(\mathbf{r}_k) \times V_k(\mathbf{r}_1, \dots, \mathbf{r}_k) \Psi(\mathbf{r}_k) \cdots \Psi(\mathbf{r}_1), \quad (1)$$

where m is the particle effective mass, $U(\mathbf{r})$ is the one-body external potential, $V_k(\mathbf{r}_1, \dots, \mathbf{r}_k)$ is a symmetric function describing k -body interactions potential, and, by neglecting the spin degree of freedom, $\Psi(\mathbf{r})$ and $\Psi^\dagger(\mathbf{r})$ are the quantized wave field operators [28] satisfying the usual relations

$$[\Psi(\mathbf{r}), \Psi(\mathbf{r}')]_{\pm} = [\Psi^\dagger(\mathbf{r}), \Psi^\dagger(\mathbf{r}')]_{\pm} = 0, \quad (2)$$

$$[\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')]_{\pm} = \delta(\mathbf{r} - \mathbf{r}'),$$

where the \pm signs refer to fermions and bosons, respectively.

Analogously, in coordinate space representation, we define the reduced density matrix [29] of a single particle (henceforth we use the symbol $\hat{}$ for single-particle operators):

$$\langle \mathbf{r} | \hat{\rho} | \mathbf{r}' \rangle = \langle \Psi^\dagger(\mathbf{r}') \Psi(\mathbf{r}) \rangle = \text{Tr}(\rho \Psi^\dagger(\mathbf{r}') \Psi(\mathbf{r})), \quad (3)$$

which in an arbitrary representation takes the usual form:

$$\langle \nu | \hat{\rho} | \nu' \rangle = \langle a_{\nu'}^\dagger a_{\nu} \rangle = \text{Tr}(\rho a_{\nu'}^\dagger a_{\nu}), \quad (4)$$

where ν, ν' are single-particle states, $a_{\nu}, a_{\nu'}^\dagger$ the annihilation and creation operators for these states, and $\langle \cdots \rangle$ the statistical mean value. In particular, in momentum space it is

$$\langle \mathbf{p} | \hat{\rho} | \mathbf{p}' \rangle = \langle a_{\mathbf{p}'}^\dagger a_{\mathbf{p}} \rangle, \quad \text{and}$$

$$\langle \mathbf{r} | \hat{\rho} | \mathbf{r}' \rangle = \frac{1}{(2\pi\hbar)^3} \int \int d^3p d^3p' e^{i\mathbf{p}\cdot\mathbf{r}} e^{-i\mathbf{p}'\cdot\mathbf{r}'} \langle a_{\mathbf{p}'}^\dagger a_{\mathbf{p}} \rangle.$$

Accordingly, for a one-particle observable $\hat{\mathcal{L}}$ we obtain as expectation value

$$\text{Tr}(\hat{\rho} \hat{\mathcal{L}}) = \int \int d^3r d^3r' \langle \Psi^\dagger(\mathbf{r}') \Psi(\mathbf{r}) \rangle \langle \mathbf{r}' | \hat{\mathcal{L}} | \mathbf{r} \rangle = \int \int d^3p d^3p' \langle a_{\mathbf{p}'}^\dagger a_{\mathbf{p}} \rangle \langle \mathbf{p}' | \hat{\mathcal{L}} | \mathbf{p} \rangle, \quad (5)$$

i.e., an *ensemble average* over many experimental realizations with a fixed number N of particles.

By using this formalism [29], we can define the *reduced* Wigner function in terms of the *reduced* density matrix (3)

$$\mathcal{F}_W = \frac{1}{(2\pi\hbar)^3} \int d^3\tau \langle \Psi^\dagger(\mathbf{r} - \tau/2) \Psi(\mathbf{r} + \tau/2) \rangle e^{-\frac{i}{\hbar} \tau \cdot \mathbf{p}}, \quad (6)$$

determining, for the momentum distribution function and for its dual expression, the relations

$$\begin{aligned} \int d^3r \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}) &= \langle a_p^\dagger a_p \rangle = \langle N_p \rangle, \\ \int d^3p \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}) &= \langle \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}) \rangle = n(\mathbf{r}), \end{aligned} \quad (7)$$

where $\langle N_p \rangle$ is the mean occupation number, $n(\mathbf{r})$ is the quasiparticle (numerical) density, and

$$\begin{aligned} \text{Tr}(\widehat{\mathcal{Q}}) &= \int \int d^3r d^3p \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}) = \int d^3p \langle a_p^\dagger a_p \rangle \\ &= \int d^3r \langle \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}) \rangle = N. \end{aligned} \quad (8)$$

Accordingly, for an arbitrary single-particle operator $\widehat{\mathcal{L}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$ that is a function of both operator $\widehat{\mathbf{r}}$ and operator $\widehat{\mathbf{p}}$, we can find a phase function [30], $\widetilde{\mathcal{L}}(\mathbf{r}, \mathbf{p})$, that *corresponds* unambiguously to operator $\widehat{\mathcal{L}}$, by introducing the Weyl-Wigner transform \mathcal{W} . In more detail, $\widetilde{\mathcal{L}}(\mathbf{r}, \mathbf{p})$ is defined by first regarding $\widehat{\mathcal{L}}$ as an integral operator with kernel $\langle \mathbf{r} | \widehat{\mathcal{L}} | \mathbf{r}' \rangle$ in the coordinate representation, and then setting

$$\widetilde{\mathcal{L}}(\mathbf{r}, \mathbf{p}) = \mathcal{W}(\widehat{\mathcal{L}}) = \int d^3\tau \langle \mathbf{r} + \boldsymbol{\tau}/2 | \widehat{\mathcal{L}} | \mathbf{r} - \boldsymbol{\tau}/2 \rangle e^{-\frac{i}{\hbar} \boldsymbol{\tau} \cdot \mathbf{p}}. \quad (9)$$

Analogously, it is possible to define the inverse Weyl-Wigner transform \mathcal{W}^{-1} (Weyl quantization), which maps the function $\widetilde{\mathcal{L}}$ on phase space into operator $\widehat{\mathcal{L}}$ on Hilbert space, so that we obtain

$$\begin{aligned} \langle \mathbf{r} | \widehat{\mathcal{L}} | \mathbf{r}' \rangle &= \mathcal{W}^{-1}(\widetilde{\mathcal{L}}) \\ &= \frac{1}{(2\pi\hbar)^3} \int d^3p \widetilde{\mathcal{L}}\left(\frac{\mathbf{r} + \mathbf{r}'}{2}, \mathbf{p}\right) e^{\frac{i}{\hbar} \mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')}. \end{aligned} \quad (10)$$

This equation defines the kernel of $\widehat{\mathcal{L}}$, and hence $\widehat{\mathcal{L}}$ itself, in terms of $\widetilde{\mathcal{L}}$. In particular, by relations (3), (6), (9), and (10) we obtain $\widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{p}) = (2\pi\hbar)^3 \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p})$ and $\langle \mathbf{r} | \widehat{\mathcal{Q}} | \mathbf{r}' \rangle = \mathcal{W}^{-1}(\widetilde{\mathcal{Q}})$.

By considering the equation of motion in the Heisenberg picture for the operator $\Psi(\mathbf{r})$, the Hamiltonian (1), the relations (2), and the symmetry property of the terms $V_k(\mathbf{r}_1, \dots, \mathbf{r}_k)$, we obtain

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}) = \mathcal{H}(\mathbf{r}) \Psi(\mathbf{r}), \quad -i\hbar \frac{\partial}{\partial t} \Psi^\dagger(\mathbf{r}) = \Psi^\dagger(\mathbf{r}) \mathcal{H}(\mathbf{r}) \quad (11)$$

with

$$\begin{aligned} \mathcal{H}(\mathbf{r}) &= -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \\ &+ \sum_{k=1}^{L-1} \frac{1}{k!} \int d^3r_1 \dots \int d^3r_k \Psi^\dagger(\mathbf{r}_1) \dots \Psi^\dagger(\mathbf{r}_k) \\ &\times V_{k+1}(\mathbf{r}, \mathbf{r}_1, \dots, \mathbf{r}_k) \Psi(\mathbf{r}_k) \dots \Psi(\mathbf{r}_1). \end{aligned} \quad (12)$$

Starting from these relations, we determine the equation of motion for the quantity $\Psi^\dagger(\mathbf{r}') \Psi(\mathbf{r})$, and by performing its statistical average we have, in the generalized Hartree approximation [31,32], the usual evolution equation for the

reduced density matrix of a single particle

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \langle \mathbf{r} | \widehat{\mathcal{Q}} | \mathbf{r}' \rangle \\ = \int d^3r'' \{ \langle \mathbf{r} | \widehat{\mathcal{H}} | \mathbf{r}'' \rangle \langle \mathbf{r}'' | \widehat{\mathcal{Q}} | \mathbf{r}' \rangle - \langle \mathbf{r} | \widehat{\mathcal{Q}} | \mathbf{r}'' \rangle \langle \mathbf{r}'' | \widehat{\mathcal{H}} | \mathbf{r}' \rangle \}, \end{aligned} \quad (13)$$

where $\widehat{\mathcal{H}} = \langle \mathcal{H} \rangle$ is the single particle Hamilton operator.

Accordingly, by applying the Fourier transform (9) to the different terms of Eq. (13) and using the inverse relation (10) to introduce the Fourier transform of $\widehat{\mathcal{H}}$ and $\widehat{\mathcal{Q}}$, we obtain

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}) \\ = \frac{1}{(2\pi\hbar)^6} \iiint d^3r' d^3p' d^3\tau d^3\phi e^{\frac{i}{\hbar} \boldsymbol{\tau} \cdot (\mathbf{p}' - \mathbf{p})} e^{\frac{i}{\hbar} \boldsymbol{\phi} \cdot (\mathbf{r} - \mathbf{r}')} \\ \times \left[\frac{p'_\alpha}{m} \phi_\alpha + V_{\text{eff}}\left(\mathbf{r}' + \frac{\boldsymbol{\tau}}{2}\right) - V_{\text{eff}}\left(\mathbf{r}' - \frac{\boldsymbol{\tau}}{2}\right) \right] \mathcal{F}_{\mathcal{W}}(\mathbf{r}', \mathbf{p}'), \end{aligned} \quad (14)$$

where

$$\begin{aligned} V_{\text{eff}}(\mathbf{r}) &= U(\mathbf{r}) + \sum_{k=1}^{L-1} \frac{1}{k!} \int d^3r_1 \dots \int d^3r_k g^{(k)}(\mathbf{r}_1, \dots, \mathbf{r}_k) \\ &\times n(\mathbf{r}_1) \dots n(\mathbf{r}_k) V_{k+1}(\mathbf{r}, \mathbf{r}_1, \dots, \mathbf{r}_k), \end{aligned} \quad (15)$$

where $g^{(k)}(\mathbf{r}_1, \dots, \mathbf{r}_k)$ is the k -order correlation function [33,34],

$$g^{(k)}(\mathbf{r}_1, \dots, \mathbf{r}_k) = \frac{\langle \Psi^\dagger(\mathbf{r}_1) \dots \Psi^\dagger(\mathbf{r}_k) \Psi(\mathbf{r}_k) \dots \Psi(\mathbf{r}_1) \rangle}{n(\mathbf{r}_1) \dots n(\mathbf{r}_k)}, \quad (16)$$

and, by construction, $g^{(1)}(\mathbf{r}_1) = 1$. Then, by expanding the term $V_{\text{eff}}(\mathbf{r}' + \boldsymbol{\tau}/2) - V_{\text{eff}}(\mathbf{r}' - \boldsymbol{\tau}/2)$ around $\boldsymbol{\tau} = 0$, we obtain (see Appendix 2) the full expansion to all orders in \hbar of the reduced Wigner equation in the generalized Hartree approximation [35],

$$\begin{aligned} \frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial t} + \frac{p_k}{m} \frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial x_k} \\ = \sum_{l=0}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \left[\frac{\partial^{2l+1} V_{\text{eff}}}{\partial x_{k_1} \dots \partial x_{k_{2l+1}}} \right] \left[\frac{\partial^{2l+1} \mathcal{F}_{\mathcal{W}}}{\partial p_{k_1} \dots \partial p_{k_{2l+1}}} \right], \end{aligned} \quad (17)$$

where Einstein convention is assumed on the saturated indices k, k_1, \dots, k_{2l+1} , and all effects of interactions are included in the definition (15) of an *effective potential*. We remark that if we consider only the first term in the sum of expression (15) (i.e., $L = 2$), then we obtain the usual Hartree approximation [36] with the two-body interactions potential

$$V_{\text{eff},2}(\mathbf{r}) = U(\mathbf{r}) + \int d^3r_1 n(\mathbf{r}_1) V_2(\mathbf{r}, \mathbf{r}_1). \quad (18)$$

On the other hand, by considering the remaining terms contained in Eq. (15) (i.e., $L > 2$), we include in $V_{\text{eff}}(\mathbf{r})$ other correction terms that are imputable to many-body interactions of higher order. Within this level of approximation, the above results can be formulated by including explicitly the spin degrees of freedom, and Eqs. (14) and (17) can be supplemented by other interaction terms. In this way the theory can be applied to a variety of physical systems, including metals, Fermi liquids [29,31], nonideal gases, and plasmas [37].

We finally note that the previous formulation describes the interactions between particles in the generalized Hartree approximation where each particle moves in the generalized average field V_{eff} produced by all the particles. Thus, the kinetic equation (17) is the exact consequence of the Heisenberg equation of motion (13) for the reduced density matrix, with $\widehat{\mathcal{H}} = \langle \mathcal{H} \rangle$ expressed by means of (12).

We notice that, by considering more carefully the interaction phenomena and, in particular, by including higher-order terms to describe the correlations between an increasing number of particles, no set of exact kinetic equations can be obtained any longer. Thus, due to the many-body nature of the problem, an infinite hierarchy of high-order density matrices (the quantum analog of the semiclassical BBGKY hierarchy [38]) can be obtained. In general, the equation of motion for an N -particle density matrix involves the $(N + 1)$ -particle density matrices, and the resulting set of kinetic equations of motion is not closed. To make the problem tractable, the central approximation stems in the truncation of the hierarchy. The truncation should occur on some level, and the successive treatment should be based on different approximation schemes, as was studied extensively for systems leading, e.g., to a semiclassical or quantum kinetic description of scattering processes [37,39,40]. Thus, taking, for example, the case of a Bose gas with contact interactions [3,41], a treatment obtained in the framework of Hartree approximation leads to Eqs. (15)–(17) and can replace the same approximations governed by a generalized Gross-Pitaevskii equation [3,5]. Analogously, to a higher order of approximation, for the same case of a Bose gas, the treatment can be generalized by introducing the quantum Boltzmann-Nordheim 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 [40].

III. DEVELOPMENT OF THE QUANTUM HYDRODYNAMIC SYSTEM IN POWERS OF \hbar

In this section we determine the relationship between the reduced Wigner function dynamics and a quantum hydrodynamic (QHD) formulation of this dynamics where one can readily derive a chain of equations of motion for an arbitrary number of macroscopic variables. Similar hydrodynamic expansions have been carried out in literature for a one-dimensional case [3,35,42]. Analogously, in the recent past, the derivation of three-dimensional QHD models, obtained by first-moments expansion [11,23,24] of the Wigner equation, has attracted considerable attention for the growing field of nanotechnology applications.

The objective of this section is to determine, in a systematic way, an extended three-dimensional QHD model, which describes the full dynamics of the generalized Wigner equation, with their classical (HD) counterpart obtained through the $\hbar \rightarrow 0$ limit. We also aim at finding the corrections to these classical models when all nonlocal effects are given not only in terms of spatial derivatives of the density, as suggested in Ref. [6], but also in terms of spatial derivatives of the temperature. In this way we determine an extended quantum hydrodynamic model that is evaluated exactly to all orders of \hbar .

A. The moments of the reduced Wigner function

By considering an arbitrary operator $\widehat{\mathcal{L}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$, and the corresponding phase-space function $\widetilde{\mathcal{L}}(\mathbf{r}, \mathbf{p})$, the macroscopic expectation value of $\widehat{\mathcal{L}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$ is given by the *global* quantity

$$\langle \widehat{\mathcal{L}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}}) \rangle = \text{Tr}(\widehat{\rho} \widehat{\mathcal{L}}) = \iint d^3 p d^3 r \widetilde{\mathcal{L}}(\mathbf{r}, \mathbf{p}) \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}, t). \quad (19)$$

Analogously, we can define the macroscopic *local moment* $F(\mathbf{r}, t)$ of $\widehat{\mathcal{L}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$ by means of the *local* relation

$$F(\mathbf{r}, t) = \int d^3 p \widetilde{\mathcal{L}}(\mathbf{r}, \mathbf{p}) \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}, t); \quad (20)$$

in this way the Wigner function acts like a joint probability distribution over position and momentum. In particular, by introducing the quantity $\varepsilon = p^2/(2m)$ and considering the group velocity $u_i = p_i/m$ as set of phase-space functions we can define the following set of traceless kinetic fields:

$$\widetilde{\mathcal{L}}_A = \{ \varepsilon^s, \varepsilon^s u_{i_1}, \varepsilon^s u_{(i_1} u_{i_2)}, \dots, \varepsilon^s u_{(i_1} u_{i_2} \dots u_{i_r)} \}, \quad (21)$$

and, by using Eq. (20), we obtain the corresponding set of *local moments*:

$$F_A(\mathbf{r}, t) = \{ F_{(s)}, F_{(s)|i_1}, F_{(s)|(i_1 i_2)}, \dots, F_{(s)|(i_1 \dots i_r)} \}, \quad (22)$$

where $s = 0, 1, \dots, \mathcal{N}$ and $r = 1, 2, \dots, M$ with \mathcal{N}, M integers labeling the maximum number of moments considered.

As in the classic extended thermodynamics approach [1], it is possible to decompose the local moments into their *convective* and *central* parts, respectively. To this purpose, we introduce the mean velocity

$$v_i = \frac{1}{n} \int d^3 p u_i \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}, t), \quad (23)$$

the peculiar velocity $\widetilde{u}_i = u_i - v_i$, and the quantity $\widetilde{\varepsilon} = \widetilde{p}^2/2m$. Thus, we consider the new set of kinetic fields

$$\widetilde{\mathcal{M}}_A = \{ \widetilde{\varepsilon}^s, \widetilde{\varepsilon}^s \widetilde{u}_{i_1}, \widetilde{\varepsilon}^s \widetilde{u}_{(i_1} \widetilde{u}_{i_2)}, \dots, \widetilde{\varepsilon}^s \widetilde{u}_{(i_1} \widetilde{u}_{i_2} \dots \widetilde{u}_{i_r)} \}, \quad (24)$$

and, in correspondence, the new set of *central moments*

$$M_A(\mathbf{r}, t) = \{ M_{(s)}, M_{(s)|i_1}, M_{(s)|(i_1 i_2)}, \dots, M_{(s)|(i_1 \dots i_r)} \}, \quad (25)$$

where, by construction,

$$M_{(0)|i_1} = 0, \quad M_{(s)|(i_1 i_2 \dots i_r)} = \int d^3 p \widetilde{\varepsilon}^s \widetilde{u}_{(i_1} \widetilde{u}_{i_2} \dots \widetilde{u}_{i_r)} \mathcal{F}_{\mathcal{W}}. \quad (26)$$

Since the vectorial moment $M_{(0)|i}$ is zero, it is replaced by the velocity v_i ; in this way there is a one-to-one correspondence between the moments F_A and the quantities $\{v_i, M_A\}$ that can be considered as the set of independent macroscopic variables. Accordingly, the total moments F_A and the central moments M_A are related by

$$F_{(s)|(i_1 \dots i_r)} = \sum_{k=0}^s \sum_{l=0}^k \sum_{q=0}^l \binom{s}{k} \binom{k}{l} \binom{l}{q} \frac{m^{s-l}}{2^{k-l}} \times v^{2(k-l)} v_{j_1} \dots v_{j_{s-k}} M_{(l)|j_1 \dots j_{s-k} (i_1 \dots i_q} v_{i_{q+1}} \dots v_{i_r}.$$

In particular, by using only an 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 $s = 0, \dots, \mathcal{N}$. Thus, for $\mathcal{N} = 0$ as

set of physical quantities we obtain the usual macroscopic variables such as the *numerical density* $n = M_{(0)}$ and the *velocity* v_i . Analogously, for $\mathcal{N} = 1$ we obtain the macroscopic variables $\{n, v_i, M_{(1)}, M_{(1)i}\}$, 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 $\mathcal{N} > 1$ we consider, as macroscopic variables, also some scalar and vectorial moments of higher order.

B. Quantum balance equations for the central moments

By multiplying Eq. (17) by $\tilde{\mathcal{M}}_A$, and integrating over the \mathbf{p} space, we determine the corresponding set of quantum balance equations (see Appendix 3) to all orders of \hbar . Thus, the balance equations for an arbitrary number of scalar and vectorial moments of the Wigner function can be expressed explicitly in the exact form as reported in Ref. [6]. In general, the closure problem of a set of balance equations can be tackled using a quantum maximum entropy formalism (QMEF) [5,6,9–11] that is formulated in its more general form in the next section.

IV. QUANTUM MAXIMUM ENTROPY PRINCIPLE

The QMEP provides the most rigorous constraint in order to select the physical constitutive equations. The maximum entropy formalism was generalized to the density-matrix formalism of quantum mechanics in a pioneer work by Jaynes [9]. In subsequent works, other authors [10] have applied the QMEP in the framework of information theory [43] and by using the Non-Equilibrium Statistical Operator Mechanics [44]. Recently the problem has been developed by considering the Weyl-Wigner formalism [5,6,11], and in this context the second-quantized formalism, in the representation of occupation numbers, is a useful starting point [45] for the incorporation of statistics into problems involving a system of identical particles.

A. Including statistics in quantum entropy

The most used definition of quantum entropy is due to Von Neumann [46] and is expressed in the form

$$S = -k_B \text{Tr}(\rho \ln \rho), \quad (27)$$

where k_B is the Boltzmann constant and ρ is the statistical density matrix operator appropriate to the physical system under study.

Although the relation (27) does not refer to any special structure of the system, there are some particular features that must be satisfied for a system of identical particles. Indeed, a main drawback of the above definition, as well as of others [11,47,48], stems from the fact that it does not include the indistinguishability principle of a system of identical particles. To account for the effects of statistics in Eq. (27), it is mandatory to consider an additional information specifying whether the density operator ρ , defined in Fock space, is associated with a fermions or bosons system.

In order to take into account *ab initio* the statistics for a system of identical particles, we can follow the Landau strategy [49] by evaluating the quantum entropy as the logarithm of the

statistical weight for the whole system. For this purpose, as shown in Refs. [5,6], for a noninteracting system of fermions or bosons in nonequilibrium conditions, the quantum entropy can be determined in terms of the functional of the reduced density matrix

$$S(\hat{\varrho}) = -k_B \text{Tr}[\hat{\Phi}(\hat{\varrho})], \quad (28)$$

where for the Fermi or Bose gases, $\hat{\Phi}(\hat{\varrho})$ is given by

$$\hat{\Phi}(\hat{\varrho}) = \hat{\varrho} \left[\ln \left(\frac{\hat{\varrho}}{y} \right) \pm y \hat{\varrho}^{-1} \left(\hat{I} \mp \frac{\hat{\varrho}}{y} \right) \ln \left(\hat{I} \mp \frac{\hat{\varrho}}{y} \right) \right], \quad (29)$$

where \hat{I} is the identity. Analogously, under nondegenerate conditions Bose and Fermi statistics tend to Boltzmann statistics as limit case, and the general expression (29) reduces to

$$\hat{\Phi}(\hat{\varrho}) = \hat{\varrho} \left[\ln \left(\frac{\hat{\varrho}}{y} \right) - \hat{I} \right] \quad (30)$$

for the Boltzmann gas.

B. General formulation of QMEP in phase space

Let us consider the operator $\hat{\mathcal{L}}_A(\hat{\mathbf{r}}, \hat{\mathbf{p}})$ with $\tilde{\mathcal{L}}_A(\mathbf{r}, \mathbf{p})$, $\langle \hat{\mathcal{L}}_A \rangle$, and $F_A(\mathbf{r}, t)$, the phase function, the expectation value, and the corresponding local moment, expressed, respectively, by relations (9), (19), and (20). In order to formulate the QMEP approach in phase space, we introduce the phase function $\hat{\Phi}(\mathbf{r}, \mathbf{p}) = \mathcal{W}(\hat{\Phi}(\hat{\varrho}))$, rewriting Eq. (28) in the form

$$S(\hat{\varrho}) = -\frac{k_B}{(2\pi\hbar)^3} \int \int d^3 p d^3 r \mathcal{W}[\hat{\Phi}(\hat{\varrho})], \quad (31)$$

and we search the extremal value of the global entropy subject to the constraint that the information on the physical system is described by a set of local moments $\{F_A(\mathbf{r}, t)\}$ with $A = 1, \dots, N$. To this purpose, we define the new *global* functional [5,6,9–11]

$$\tilde{S} = S - \int d^3 r \left[\sum_{A=1}^N \tilde{\lambda}_A \left(\int d^3 p \tilde{\mathcal{L}}_A \mathcal{F}_W - F_A \right) \right], \quad (32)$$

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

$$\hat{\Phi}(\hat{\varrho}) = \mathcal{W}^{-1} \left(- \sum_{A=1}^N \lambda_A \tilde{\mathcal{L}}_A \right), \quad (33)$$

with $\lambda_A = \tilde{\lambda}_A/k_B$. In particular, if we use the set (24) as kinetic fields, the corresponding central moments (25) as constraints, and the explicit expressions (29) and (30) for the function $\hat{\Phi}(\hat{\varrho})$, then, by relation (33), we obtain the following:

(i) In the case of Fermi and Bose statistics, the functional form [5,6]

$$\hat{\varrho} = y \left(\exp \left\{ \mathcal{W}^{-1} \left[\sum_{A=1}^N \lambda_A(\mathbf{r}, t) \tilde{\mathcal{M}}_A \right] \right\} \pm \hat{I} \right)^{-1}. \quad (34)$$

(ii) In the case of Boltzmann statistics, the simplified expression

$$\hat{q} = y \exp \left\{ \mathcal{W}^{-1} \left[- \sum_{A=1}^N \lambda_A(\mathbf{r}, t) \tilde{\mathcal{M}}_A \right] \right\}. \quad (35)$$

Thus, by applying the Fourier transform (9), the reduced Wigner function takes the form

$$\mathcal{F}_W = \frac{1}{(2\pi\hbar)^3} \mathcal{W}(\hat{q}[\lambda_A(\mathbf{r}, t), \tilde{\mathcal{M}}_A]). \quad (36)$$

We stress that, in the set of quantum hydrodynamic equations (A19) and (A20) reported in Appendix 3, the effects of interactions are entirely contained in $V_{\text{eff}}(\mathbf{r})$.

Accordingly, 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 dynamical evolution of the system, but it offers only a definite procedure to construct a sequence of approximations for the nonequilibrium 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 and (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 among particles. Thus, by knowing the functional form (34)–(36) of the reduced Wigner function, we use Eq. (17) to obtain a set of evolution equations for the constraints. This set completely represents the QHD model (A19) and (A20) reported in the Appendix, 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.

V. MOYAL EXPANSION OF THE WIGNER FUNCTION

By using the Moyal formalism [50] one can prove [45,51,52] that the Wigner function, and consequently the central moments, can be expanded in even powers of \hbar as

$$\mathcal{F}_W = \sum_{k=0}^{\infty} \hbar^{2k} \mathcal{F}_W^{(2k)}, \quad M_A = \sum_{k=0}^{\infty} \hbar^{2k} M_A^{(2k)}. \quad (37)$$

With this approach, we obtain a system in which the dynamical evolution is described by resolving, order by order, a closed hydrodynamic 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

$$M_A = \frac{1}{(2\pi\hbar)^3} \int d^3 p \tilde{\mathcal{M}}_A \mathcal{W}(\hat{q}[\lambda_A(\mathbf{r}, t), \tilde{\mathcal{M}}_A]). \quad (38)$$

The inversion problem can be solved only by assuming that also the Lagrange multipliers can be expanded in even powers of \hbar . Thus, we search λ_A in the form [5,6]

$$\lambda_A(\mathbf{r}, t) = \sum_{r=0}^{\infty} \hbar^{2r} \lambda_A^{(2r)}(\mathbf{r}, t), \quad (39)$$

with the condition that for $\hbar \rightarrow 0$ we determine the usual expressions for both the Lagrange multipliers and the distribution function obtained in the framework of the classic MEP approach [1,7]. In particular, under local equilibrium conditions we obtain the usual Maxwell-Boltzmann distribution function for nondegenerate gases, and the usual Bose or Fermi distribution functions for degenerate gases.

In the next sections, the Moyal formalism is applied to develop a nonlocal theory for the Fermi and Bose gases, which is evaluated explicitly, up to the first quantum correction. However, it is worth noting that, hereafter, all the results concerning Boltzmann statistics will be determined as a limit case of Fermi and Bose statistics.

A. Moyal and quasi-Moyal approximations for the Fermi and Bose gases

By following the approach reported in Appendix 5, we consider the Weyl-Wigner transform of the density operator (34). Thus, in the framework of Fermi and Bose statistics, we obtain for the Wigner function the expansion [6]

$$\mathcal{F}_W = \frac{\tilde{y}}{e^{\Pi} \pm 1} \left(1 + \sum_{r=1}^{\infty} \hbar^{2r} P_{2r}^{\pm} \right), \quad \text{with} \quad (40)$$

$$\Pi = \sum_{A=1}^N \lambda_A \tilde{\mathcal{M}}_A,$$

where \tilde{y} and the quantities P_{2r}^{\pm} are explicitly expressed in Appendix 5.

We remark that the present strategy generalizes all the results reported in literature for a quantum gas [23–27]. In particular, by considering the different terms P_{2r}^{\pm} of expansion (40) we generalize some recent results reported in Ref. [6] by obtaining a sequence of approximate solutions (quasi-Moyal approximations), where, on a macroscopic scale, all the nonlocal effects are captured not only in terms of spatial derivatives of the density but also in terms of spatial derivatives of the temperature.

At this stage, the Lagrange multipliers λ_A can be determined using an *iterative procedure* and inverting the relations (38) evaluated up to a given order in power of \hbar^2 .

Accordingly, in the zero-order approximation, we assume

$$\mathcal{F}_W \approx \frac{\tilde{y}}{e^{\Pi} \pm 1}, \quad \text{with} \quad M_A + O(\hbar^2) = \int d^3 p \tilde{\mathcal{M}}_A \mathcal{F}_W, \quad (41)$$

where the moments M_A are the classic macroscopic variables, and, consequently, the Lagrange multipliers λ_A must be determined as solutions of relations (41)₂. In this way, we obtain the classic nonequilibrium relations

$$\begin{aligned} \lambda_A &= \lambda_A(M_B) + O(\hbar^2), \\ \mathcal{F}_W &= \mathcal{F}_W(M_A, \tilde{\mathbf{p}}) + O(\hbar^2), \\ H_A &= H_A(M_B) + O(\hbar^2). \end{aligned} \quad (42)$$

Analogously, the first-order quantum approximation is obtained by considering the successive term of the series (40),

i.e., the quasi-Moyal expression

$$\mathcal{F}_{\mathcal{W}} \approx \frac{\tilde{y}}{e^{\Pi} \pm 1} (1 + \hbar^2 P_2^{\pm}), \quad \text{with} \quad \Pi = \sum_{A=1}^N \lambda_A \tilde{\mathcal{M}}_A, \quad (43)$$

where, by using the previous iteration, the term P_2^{\pm} is expressed in the form

$$P_2^{\pm} = P_2^{\pm} \left(M_B, \frac{\partial M_B}{\partial x_k}, \frac{\partial^2 M_B}{\partial x_i \partial x_k}, \tilde{\mathbf{p}} \right) + O(\hbar^2). \quad (44)$$

By following this approach, the first quantum approximation for λ_A , is obtained by inverting the relations

$$M_A + O(\hbar^4) = \int d^3 p \tilde{\mathcal{M}}_A \mathcal{F}_{\mathcal{W}}, \quad (45)$$

where, in the course of this computation, we assume that the quantities M_A are evaluated up to the first-order quantum correction. Then we formally obtain

$$\lambda_A = \lambda_A \left(M_B, \frac{\partial M_B}{\partial x_k}, \frac{\partial^2 M_B}{\partial x_i \partial x_k} \right) + O(\hbar^4), \quad (46)$$

and, consequently, both the Wigner function and the constitutive functions H_A are estimated, by means of expressions (43)–(46) and (A24), in the form

$$\mathcal{F}_{\mathcal{W}} = \mathcal{F}_{\mathcal{W}} \left(M_A, \frac{\partial M_A}{\partial x_k}, \frac{\partial^2 M_A}{\partial x_i \partial x_k}, \tilde{\mathbf{p}} \right) + O(\hbar^4), \quad (47)$$

$$H_A = H_A \left(M_B, \frac{\partial M_B}{\partial x_k}, \frac{\partial^2 M_B}{\partial x_i \partial x_k} \right) + O(\hbar^4). \quad (48)$$

The advantage of this approach is that, to every quantum approximation, we obtain the Lagrange multipliers using the previous iterations and by inverting order by order the relations (38). Thus, both the Lagrange multipliers and the constitutive relations are determined as functions both of moments and their spatial derivatives up to the prefixed order in power of \hbar^2 . We conclude by remarking that, formally, Eq. (43)₁ should be considered as a *quasi-Moyal approximation* of the Wigner function, since to obtain an effective Moyal-approximation up to terms of order \hbar^2 , also an expansion of term $[e^{\Pi} \pm 1]^{-1}$ should be explicitly considered.

In the following we adopt the above strategy by using the set (24) of kinetic fields and the set (26) of corresponding moments. Generally, the inversion of relations (45) is a rather complicate procedure owing to the nonlinearity of \mathcal{F} with respect to the Lagrange multipliers. However, the inversion can be performed by using a more affordable series expansion around some local equilibrium configuration. In the next section we consider this approach and develop, explicitly, the series expansion by using only an arbitrary set of scalar and vectorial moments of the distribution function.

VI. EXPANSION OF THE WIGNER FUNCTION AROUND LOCAL EQUILIBRIUM

To determine an analytical expression of the Wigner function, through the relations (43)₁, it is necessary to obtain an explicit representation of λ_A . To this purpose, we consider only the kinetic fields $\tilde{\mathcal{M}}_A = \{\tilde{\varepsilon}^l, \tilde{\varepsilon}^l \tilde{u}_i\}$ and decompose the Lagrange multipliers in the equilibrium and nonequilibrium local parts [6] where $\{\alpha(\mathbf{r}, t), \beta(\mathbf{r}, t)\}$ are the nonvanishing Lagrange multipliers of local equilibrium, while $\Lambda_A(\mathbf{r}, t) = \{\Lambda_{(l)}, \Lambda_{(l)i}\}$ are the nonequilibrium Lagrange multipliers with

$$\alpha = \sum_{k=0}^{\infty} \hbar^{2k} \alpha^{(2k)}, \quad \beta = \sum_{k=0}^{\infty} \hbar^{2k} \beta^{(2k)}, \quad \Lambda_A = \sum_{k=0}^{\infty} \hbar^{2k} \Lambda_A^{(2k)}. \quad (49)$$

With this procedure, we can consider an expansion [6] of the relation (43)₁ up to first order with respect to the deviations from the local equilibrium configuration $\mathcal{F}_{\mathcal{W}|E}$

$$\mathcal{F}_{\mathcal{W}} \approx \mathcal{F}_{\mathcal{W}|E} + \sum_{A=1}^N \left(\frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial \Lambda_A} \right)_E \Lambda_A, \quad (50)$$

by assuming, in the course of this computation, that all the terms associated with the spatial variations of $\Lambda_A^{(0)}$ are negligible with respect to the terms connected with the spatial variations of the equilibrium quantity $\alpha^{(0)}$ and $\beta^{(0)}$. With this assumption, the analytical computation becomes significantly simpler, and the nonlocal effects expressed by the quantum correction of the Wigner function should be ascribed essentially to the spatial derivatives of both density n and effective temperature T .

A. Nonlocal expansion for Fermi and Bose gases

By expanding the quasi-Moyal approximation (43)₁ in terms of the nonequilibrium Lagrange multipliers Λ_A , we obtain the *equilibrium* and the linear *nonequilibrium* contributions of $\mathcal{F}_{\mathcal{W}}$ (see Appendix 6)

$$\mathcal{F}_{\mathcal{W}|E} = \tilde{y} (L_{(0)}^{\pm} + \hbar^2 P_2^{\pm(0)}), \quad (51)$$

$$\mathcal{F}_{\mathcal{W}|NE} = \tilde{y} (L_{(1)}^{\pm} + \hbar^2 P_2^{\pm(1)}) \times \left(\sum_{l=0}^N \Lambda_{(l)} \tilde{\varepsilon}^l + \sum_{l=0}^N \Lambda_{(l)i} \tilde{\varepsilon}^l \tilde{u}_i \right), \quad (52)$$

where $\tilde{y} = (2\tilde{s} + 1)/(2\pi\hbar)^3$ (with $\tilde{s}\hbar$ the particle spin), the functions $L_{(n)}^{\pm}$ are given by

$$L_{(n)}^{\pm} = \frac{d^n}{d\alpha^n} \left(\frac{1}{e^{\alpha + \beta \tilde{\varepsilon}} \pm 1} \right), \quad (53)$$

and the quantum correction terms $\{P_2^{\pm(0)}, P_2^{\pm(1)}\}$ will be expressed in the following form:

$$P_2^{\pm(r)} = \frac{1}{12m} \frac{1}{k_B T} \left\{ [L_{(3+r)}^{\pm} \mathcal{Q}^{(1,1)} + L_{(2+r)}^{\pm} \mathcal{Q}^{(2,1)}] + \frac{m}{k_B T} [L_{(3+r)}^{\pm} \mathcal{Q}^{(1,2)} + L_{(2+r)}^{\pm} \mathcal{Q}^{(2,2)}] \tilde{u}^2 + \left(\frac{m}{k_B T} \right)^2 L_{(3+r)}^{\pm} \mathcal{Q}^{(1,3)} \tilde{u}^4 \right. \\ \left. + \frac{m}{k_B T} [L_{(3+r)}^{\pm} \mathcal{Q}_{(ij)}^{(1,4)} + L_{(2+r)}^{\pm} \mathcal{Q}_{(ij)}^{(2,4)}] \tilde{u}_i \tilde{u}_j + \left(\frac{m}{k_B T} \right)^2 L_{(3+r)}^{\pm} \mathcal{Q}_{(ij)}^{(1,5)} \tilde{u}^2 \tilde{u}_i \tilde{u}_j \right\} + O(\hbar^2) \quad \text{for } r = 0, 1, \quad (54)$$

where the nonlocal quantities $\{Q^{(k,l)}\}$ and $\{Q_{(ij)}^{(k,l)}\}$ are explicitly reported in Eqs. (A70)–(A77) of the Appendix in terms of $\{n, T, \frac{\partial n}{\partial x_k}, \frac{\partial T}{\partial x_k}, \frac{\partial^2 n}{\partial x_i \partial x_k}, \frac{\partial^2 T}{\partial x_i \partial x_k}\}$ and of Fermi and Bose integral functions $I_n^\pm(\alpha)$ defined in Eqs. (A68) and (A69).

1. The density-gradient approximation

It should be noted that, in general, if the spatial derivatives of the effective temperature $T(\mathbf{r}, t)$ are very large in the regions where also the numerical density $n(\mathbf{r}, t)$ varies very quickly, then nonlocal effects imputable to the temperature cannot be neglected. By contrast, if all the terms associated with temperature gradient are negligible with respect to terms connected with the density gradient, then we obtain the usual nonlocal effects [5,6,23–27] imputable only to the spatial derivatives of the numerical density [53]. In this case the quantities $\{Q^{(2,2)}, Q^{(1,3)}, Q_{(ij)}^{(2,4)}, Q_{(ij)}^{(1,5)}\}$ can be neglected in Eq. (54), and the remaining terms will admit for a simplified expression. Consequently, we reobtain some recent results reported in Ref. [6], and the quantum correction terms $P_2^{\pm(r)}$ take the simplified form

$$P_2^{\pm(r)} = \frac{1}{12m} \frac{1}{k_B T} \left\{ [L_{(3+r)}^\pm Q^{(1)} + 9L_{(2+r)}^\pm Q^{(2)}] + \frac{m}{k_B T} L_{(3+r)}^\pm [Q^{(2)} \tilde{u}^2 + Q_{(ij)} \tilde{u}_i \tilde{u}_j] \right\} + O(\hbar^2) \quad (55)$$

for $r = 0, 1$,

where the nonlocal quantities $\{Q^{(k)}, Q_{(ij)}\}$ can be obtained, by using the relations (A78), only as functions of $\{n, T, \frac{\partial n}{\partial x_k}, \frac{\partial^2 n}{\partial x_i \partial x_k}\}$.

B. Nonlocal expansion for a Boltzmann gas

We remark that for $\alpha \gg 1$ both Bose and Fermi statistics tend to Boltzmann statistic. As a consequence, from expressions (51)–(54) we obtain (see Appendix 7) the following explicit *equilibrium* and linear *nonequilibrium* contributions for a Boltzmann gas:

$$\begin{aligned} \mathcal{F}_{W|E} &= \tilde{y} e^{-\alpha} e^{-\beta \tilde{\varepsilon}} \{1 + \hbar^2 \tilde{Q}_2\}, \quad (56) \\ \mathcal{F}_{W|NE} &= -\tilde{y} e^{-\alpha} e^{-\beta \tilde{\varepsilon}} \{1 + \hbar^2 \tilde{Q}_2\} \\ &\quad \times \left\{ \sum_{l=0}^N \Lambda_{(l)} \tilde{\varepsilon}^l + \sum_{l=0}^N \Lambda_{(l)i} \tilde{\varepsilon}^l \tilde{u}_i \right\}, \quad (57) \end{aligned}$$

where the quantum correction term \tilde{Q}_2 is expressed in the form

$$\begin{aligned} \tilde{Q}_2 &= \frac{1}{12m} \frac{1}{k_B T} \left\{ Q^{(1)} + \frac{m}{k_B T} Q^{(2)} \tilde{u}^2 + \left(\frac{m}{k_B T} \right)^2 Q^{(3)} \tilde{u}^4 \right. \\ &\quad \left. + \frac{m}{k_B T} Q_{(ij)}^{(4)} \tilde{u}_i \tilde{u}_j + \left(\frac{m}{k_B T} \right)^2 Q_{(ij)}^{(5)} \tilde{u}^2 \tilde{u}_i \tilde{u}_j \right\} + O(\hbar^2), \quad (58) \end{aligned}$$

and the quantities $\{Q^{(1)}, Q^{(2)}, Q^{(3)}, Q_{(ij)}^{(4)}, Q_{(ij)}^{(5)}\}$ are nonlocal functions of $\{n, T, \frac{\partial n}{\partial x_k}, \frac{\partial T}{\partial x_k}, \frac{\partial^2 n}{\partial x_i \partial x_k}, \frac{\partial^2 T}{\partial x_i \partial x_k}\}$ that can be obtained by using of relations (A91) and (A92).

Also in this case, if we consider the *density-gradient approximation*, then it is possible to neglect all terms containing the spatial derivatives of temperature in Eq. (58). In

particular, $Q^{(3)}$ and $Q_{(ij)}^{(5)}$ can be neglected, while the remaining quantities $\{Q^{(1)}, Q^{(2)}, Q_{(ij)}^{(4)}\}$ are expressed only as function of $\{n, \frac{\partial n}{\partial x_k}, \frac{\partial^2 n}{\partial x_i \partial x_k}\}$, and the quantum correction term \tilde{Q}_2 takes the simplified explicit form

$$\begin{aligned} \tilde{Q}_2 &= \frac{1}{24m} \frac{1}{k_B T} \left\{ \left[3 \frac{\partial^2 \ln n}{\partial x_k \partial x_k} + \left(\frac{\partial \ln n}{\partial x_k} \right)^2 \right] \right. \\ &\quad \left. - \frac{m}{k_B T} \frac{\partial^2 \ln n}{\partial x_i \partial x_j} \tilde{u}_i \tilde{u}_j \right\} + O(\hbar^2). \quad (59) \end{aligned}$$

VII. LAGRANGE MULTIPLIERS AND CLOSURE RELATIONS IN EQUILIBRIUM CONDITIONS

By inserting the quasi-Moyal approximation (51) into the definition of the macroscopic quantities (45), we can determine the equilibrium Lagrange multipliers. As a consequence, through Eq. (26)₂, also the constitutive functions (A24) can be obtained in equilibrium conditions up to the first quantum correction with respect to the classic expressions.

A. Quantum chemical potential and quantum equation of state

By using the approximation (51), we can calculate the variables of local equilibrium $n(\mathbf{r}, t) = M_{(0)}(\mathbf{r}, t)$ and $P(\mathbf{r}, t) = 2/3 M_{(1)}(\mathbf{r}, t)$ through the relations

$$n(\mathbf{r}, t) + O(\hbar^4) = \int d^3 p \mathcal{F}_{W|E}, \quad (60)$$

$$P(\mathbf{r}, t) + O(\hbar^4) = \frac{2}{3} \int d^3 p \tilde{\varepsilon} \mathcal{F}_{W|E}, \quad (61)$$

where $\{n(\mathbf{r}, t), P(\mathbf{r}, t)\}$ are evaluated up to the first-order quantum correction. In particular, by assuming $\beta = (k_B T)^{-1}$ and introducing the dimensionless quantities

$$\eta_{ij}^{(s)} = 2^{j-1} (-1)^i \frac{\Gamma(s + j + \frac{1}{2})}{\Gamma(s + j + i - \frac{7}{2})} \frac{I_{2(s+j+i-4)}^\pm}{I_{2(s+1)}^\pm} \quad (62)$$

with s, i, j integer, we determine the following generalized *differential constraints* for the QHD system:

$$\begin{aligned} I_2^\pm(\alpha) &= \gamma \frac{n}{T^{3/2}} \left\{ 1 - \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[\sum_{p=1}^3 \eta_{1p}^{(0)} Q^{(1,p)} \right. \right. \\ &\quad \left. \left. + \sum_{q=1}^2 \eta_{2q}^{(0)} Q^{(2,q)} \right] \right\} + O(\hbar^4), \quad (63) \end{aligned}$$

$$\begin{aligned} P &= \frac{2}{3} n k_B T \frac{I_4^\pm}{I_2^\pm} \left\{ 1 + \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[\sum_{p=1}^3 (\eta_{1p}^{(1)} - \eta_{1p}^{(0)}) Q^{(1,p)} \right. \right. \\ &\quad \left. \left. + \sum_{q=1}^2 (\eta_{2q}^{(1)} - \eta_{2q}^{(0)}) Q^{(2,q)} \right] \right\} + O(\hbar^4), \quad (64) \end{aligned}$$

where $\gamma^{-1} = [4(2\tilde{s} + 1)/\sqrt{\pi}] (mk_B/2\pi\hbar^2)^{3/2}$.

Accordingly, by solving the relation (63) with respect to α , we determine the quantum *chemical potential* $\mu = -\alpha k_B T$, while by using Eq. (64) we obtain the generalized quantum equation of state for the system under interest. We remark that, in general, the *differential constraints* (63) and (64) should

be solved numerically step by step with every set of closed QHD equations. In this way, it is possible to determine both the Lagrange multiplier α and the pressure P as numerical nonlocal functions of variables n and T .

In this section we generalize the procedure reported in Ref. [6] by assuming that the nonlocal effect are imputable to the spatial derivatives of both density n and temperature T . Thus, for various degeneracy levels of Fermi and Bose gases, some simplified analytical cases can be analyzed.

1. Completely nondegenerate Fermi and Bose gases

For the case $\alpha \gg 1$, we use only the first term of a suitable expansion in series for the Fermi and Bose integral functions [6,54]. Accordingly, we take $I_n^\pm(\alpha) \approx (1/2)\Gamma[(n+1)/2] \exp(-\alpha)$, and by using Eqs. (62)–(64) and (A70)–(A74) obtain the following relations:

$$\begin{aligned}\mu &= k_B T \ln [\chi^{(0)}] + \frac{Q_B^I}{3} + O(\hbar^4), \\ P &= n k_B T + n Q_C^I + O(\hbar^4),\end{aligned}\quad (65)$$

where $\chi^{(0)} = (4\gamma/\sqrt{\pi})n/T^{3/2} \ll 1$ and the quantum corrections terms are expressed in the form

$$\begin{aligned}Q_B^I &= -\frac{\hbar^2}{8m} \left\{ 2 \frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \left(\frac{\partial \ln n}{\partial x_r} \right)^2 - \frac{\partial^2 \ln T}{\partial x_r \partial x_r} \right. \\ &\quad \left. + \frac{1}{2} \left(\frac{\partial \ln T}{\partial x_r} \right)^2 - 2 \frac{\partial \ln n}{\partial x_r} \frac{\partial \ln T}{\partial x_r} \right\},\end{aligned}\quad (66)$$

$$\begin{aligned}Q_C^I &= -\frac{\hbar^2}{36m} \left\{ \frac{\partial^2 \ln n}{\partial x_r \partial x_r} - \frac{\partial^2 \ln T}{\partial x_r \partial x_r} \right. \\ &\quad \left. + \frac{1}{2} \left(\frac{\partial \ln T}{\partial x_r} \right)^2 - \frac{\partial \ln n}{\partial x_r} \frac{\partial \ln T}{\partial x_r} \right\}.\end{aligned}\quad (67)$$

We remark that the relations (65)–(67) generalize all the results known in literature in the framework of Wigner theory for a Boltzmann gas [6]. In particular, if we assume that the nonlocal effects are imputable to both the spatial derivatives of density n and temperature T , then the terms Q_B^I and Q_C^I represent, respectively, the natural generalization of the usual Bohm quantum potential $Q_B = -(\hbar^2/2m\sqrt{n})\Delta\sqrt{n}$, and of the usual quantum correction for the pressure P . Indeed if, for the sake of simplicity, we consider the usual *density-gradient approximation* [5,6,23,24,53], we find $Q_B^I \approx Q_B$ and $Q_C^I \approx -(\hbar^2/36m)\Delta \ln n$. Consequently, by using Eqs. (65) we recover the well-known results for the chemical potential [23] and for the pressure [24] in the case of the quantum Boltzmann gas [6].

2. Weakly degenerate Fermi and Bose gases

In the case $\alpha > 1$, the statistics corresponds to that of a weakly degenerate gas. Thus, by using the first two terms in a series expansion [6,54] $I_n^\pm(\alpha) \approx (1/2)\Gamma[(n+1)/2] \exp(-\alpha)\{1 \mp \exp(-\alpha/2^{(n+1)/2})\}$, and by considering the usual iterative procedure [6,49,54], we use Eqs. (62)–(64) and

(A70)–(A74) up to order \hbar^2 , to obtain the first statistical corrections in terms of quantity $\chi^{(0)} \ll 1$, where

$$\begin{aligned}\mu &= k_B T \ln \left[\left(1 \pm \frac{\chi^{(0)}}{2^{3/2}} \right) \chi^{(0)} \right] \\ &\quad + \frac{1}{3} \left(Q_B^I \pm \frac{\chi^{(0)}}{2^{3/2}} Q_B^{II} \right) + O(\hbar^4),\end{aligned}\quad (68)$$

$$P = n k_B T \left(1 \pm \frac{\chi^{(0)}}{2^{5/2}} \right) + n \left(Q_C^I \mp \frac{\chi^{(0)}}{2^{5/2}} Q_C^{II} \right) + O(\hbar^4),\quad (69)$$

where the quantum statistical corrections Q_B^{II} , Q_C^{II} are expressed in the form

$$\begin{aligned}Q_B^{II} &= -\frac{\hbar^2}{8m} \left\{ -2 \frac{\partial^2 \ln n}{\partial x_r \partial x_r} - 2 \left(\frac{\partial \ln n}{\partial x_r} \right)^2 + 3 \frac{\partial^2 \ln T}{\partial x_r \partial x_r} \right. \\ &\quad \left. - 3 \left(\frac{\partial \ln T}{\partial x_r} \right)^2 + 5 \frac{\partial \ln n}{\partial x_r} \frac{\partial \ln T}{\partial x_r} \right\},\end{aligned}\quad (70)$$

$$\begin{aligned}Q_C^{II} &= -\frac{\hbar^2}{36m} \left\{ 6 \frac{\partial^2 \ln n}{\partial x_r \partial x_r} + 7 \left(\frac{\partial \ln n}{\partial x_r} \right)^2 - 9 \frac{\partial^2 \ln T}{\partial x_r \partial x_r} \right. \\ &\quad \left. + \frac{45}{4} \left(\frac{\partial \ln T}{\partial x_r} \right)^2 - 18 \frac{\partial \ln n}{\partial x_r} \frac{\partial \ln T}{\partial x_r} \right\}.\end{aligned}\quad (71)$$

Also in this case, if we assume that nonlocal effects are imputable only to the spatial derivatives of density n (i.e., the *density-gradient approximation*), then we can neglect all terms containing the spatial derivatives of temperature, and we reobtain, for μ and P , the results explicitly reported in Ref. [6] in the weakly degenerate case.

3. Completely degenerate Fermi gases

For the Fermi statistics under strong degeneracy we can use the asymptotic Sommerfeld expansion [49,54–56] for the functions $I_n^+(\alpha)$. In particular, for $\alpha \ll -1$ the degeneracy becomes complete, and we can use the approximation $I_n^+(\alpha) \approx (-\alpha)^{(n+1)/2}/(n+1)$. In this case, we assume that $T \rightarrow 0$ and $\partial T/\partial x_k \rightarrow 0$; consequently the nonlocal effect can be imputable only to the spatial derivatives of density n , and we obtain [6] for μ and P

$$\begin{aligned}\mu &= \frac{5}{2} v_F n^{2/3} + \frac{Q_B}{9} + O(\hbar^4), \\ P &= v_F n^{5/3} + \frac{\hbar^2}{36m} \left\{ \frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \frac{4}{3} \left(\frac{\partial \ln n}{\partial x_r} \right)^2 \right\} + O(\hbar^4),\end{aligned}\quad (72)$$

where $v_F = (\hbar^2/5m)[6\pi^2/(2\tilde{s}+1)]^{2/3}$. Also in this case, we recover the well-known results obtained, using the density-gradient functional formalism for the Fermi gas [57], when $T \rightarrow 0$.

4. Strongly degenerate Fermi gases

For $\alpha \ll -1$ and $T > 0$ we can use the first two terms of the asymptotic Sommerfeld expansion obtaining for $I_n^+(\alpha) \approx [(-\alpha)^{(n+1)/2}/(n+1)]\{1 + (\pi^2/24)(n^2-1)(-\alpha)^{-2}\}$. Accordingly, by considering the usual iterative procedure [6], we define $\mu^{(0)} = (5v_F/2)n^{2/3}$ and, using Eqs. (62)–(64) and (A70)–(A74) up to order \hbar^2 , we determine the quantum statistical corrections in terms of quantities $(k_B T/\mu^{(0)})^2 \ll 1$.

In this case we assume that, in general for $T > 0$, the nonlocal effects can be imputable to both the spatial derivatives of density n and of temperature T . Thus, we obtain

$$\mu = \mu^{(0)} \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\mu^{(0)}} \right)^2 \right] + \frac{1}{9} \left[Q_D^I + \frac{\pi^2}{12} \left(\frac{k_B T}{\mu^{(0)}} \right)^2 Q_D^{II} \right] + O(\hbar^4), \quad (73)$$

$$P = \nu_F n^{5/3} \left[1 + \frac{5}{12} \pi^2 \left(\frac{k_B T}{\mu^{(0)}} \right)^2 \right] + n \left[Q_E^I + \frac{\pi^2}{3} \left(\frac{k_B T}{\mu^{(0)}} \right)^2 Q_E^{II} \right] + O(\hbar^4), \quad (74)$$

where

$$Q_D^I = -\frac{\hbar^2}{8m} \left\{ 2 \frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \left(\frac{\partial \ln n}{\partial x_r} \right)^2 + 3 \frac{\partial^2 \ln T}{\partial x_r \partial x_r} - 2 \frac{\partial \ln n}{\partial x_r} \frac{\partial \ln T}{\partial x_r} \right\}, \quad (75)$$

$$Q_D^{II} = -\frac{\hbar^2}{8m} \left\{ 8 \frac{\partial^2 \ln n}{\partial x_r \partial x_r} - \frac{4}{3} \left(\frac{\partial \ln n}{\partial x_r} \right)^2 - 18 \frac{\partial^2 \ln T}{\partial x_r \partial x_r} - 9 \left(\frac{\partial \ln T}{\partial x_r} \right)^2 + 12 \frac{\partial \ln n}{\partial x_r} \frac{\partial \ln T}{\partial x_r} \right\}, \quad (76)$$

$$Q_E^I = \frac{\hbar^2}{36m} \left\{ \frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \frac{4}{3} \left(\frac{\partial \ln n}{\partial x_r} \right)^2 - 2 \frac{\partial^2 \ln T}{\partial x_r \partial x_r} + \left(\frac{\partial \ln T}{\partial x_r} \right)^2 - 2 \frac{\partial \ln n}{\partial x_r} \frac{\partial \ln T}{\partial x_r} \right\}, \quad (77)$$

$$Q_E^{II} = \frac{\hbar^2}{36m} \left\{ -\frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \frac{9}{5} \frac{\partial^2 \ln T}{\partial x_r \partial x_r} + \frac{3}{4} \left(\frac{\partial \ln T}{\partial x_r} \right)^2 - \frac{7}{10} \frac{\partial \ln n}{\partial x_r} \frac{\partial \ln T}{\partial x_r} \right\}. \quad (78)$$

Also in this case, by assuming the *density-gradient approximation* we can neglect all terms containing the spatial derivatives of temperature in the previous relations, and we reobtain the results reported in Ref. [6] for the chemical potential μ and for the pressure P in the strongly degenerate case.

B. Moments and closure relations in equilibrium conditions

From equation (60), we calculate the remaining moments in the equilibrium conditions, through the following relationships:

$$M_{(s)}|_E = \int d^3 p \tilde{\varepsilon}^s \mathcal{F}_{\mathcal{W}}|_E + O(\hbar^4), \quad s \geq 2, \quad (79)$$

$$M_{(s)|(i_1 i_2 \dots i_r)}|_E = \int d^3 p \tilde{\varepsilon}^s \tilde{u}_{i_1} \tilde{u}_{i_2} \dots \tilde{u}_{i_r} \mathcal{F}_{\mathcal{W}}|_E + O(\hbar^4), \quad s \geq 0. \quad (80)$$

Thus, we obtain

$$M_{(s)}|_E = n \frac{I_{2(s+1)}^\pm}{I_2^\pm} (k_B T)^s \left\{ 1 + \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[\sum_{p=1}^3 (\eta_{1p}^{(s)} - \eta_{1p}^{(0)}) \mathcal{Q}^{(1,p)} + \sum_{q=1}^2 (\eta_{2q}^{(s)} - \eta_{2q}^{(0)}) \mathcal{Q}^{(2,q)} \right] \right\} + O(\hbar^4), \quad s \geq 2, \quad (81)$$

$$M_{(s)|(ij)}|_E = \hbar^2 \frac{2}{45} \frac{n}{m^2} (k_B T)^s \left\{ -\frac{\Gamma(s + \frac{7}{2})}{\Gamma(s + \frac{1}{2})} \frac{I_{2s}^\pm}{I_2^\pm} \mathcal{Q}_{(ij)}^{(1,4)} + \frac{\Gamma(s + \frac{7}{2})}{\Gamma(s + \frac{3}{2})} \frac{I_{2(s+1)}^\pm}{I_2^\pm} \mathcal{Q}_{(ij)}^{(2,4)} - 2 \frac{\Gamma(s + \frac{9}{2})}{\Gamma(s + \frac{3}{2})} \frac{I_{2(s+1)}^\pm}{I_2^\pm} \mathcal{Q}_{(ij)}^{(1,5)} \right\} + O(\hbar^4), \quad s \geq 0, \quad (82)$$

and analogously

$$M_{(s)}|_i = 0 + O(\hbar^4), \quad M_{(s)|(i_1 i_2 \dots i_r)}|_E = 0 + O(\hbar^4) \quad \text{with } s \geq 0 \quad \text{and } r \geq 3. \quad (83)$$

It should be noted that, having considered the relations (60) and (61) to determine both α and the equation of state, then two degrees of freedom for the remaining system are lost. Consequently, the scalar moments $M_{(s)}$ have been evaluated only for $s \geq 2$ because, using the relations (81) with $s = 0, 1$, we reobtain, respectively, the density n and the quantum expression (64) for pressure P . Finally, by assuming as further condition the *density-gradient approximation*, then all quantities $\{\mathcal{Q}^{(1,3)}, \mathcal{Q}^{(2,2)}, \mathcal{Q}_{(ij)}^{(2,4)}, \mathcal{Q}_{(ij)}^{(1,5)}\}$ can be neglected in Eqs. (81) and (82), and, by considering the relations (A78), a simplified expression for $\{M_{(s)}|_E, M_{(s)|(ij)}|_E\}$ is determined.

1. Boltzmann statistics as limit case

Being expressed in terms of Fermi and Bose integral functions, the previous relations are valid for arbitrary values of α . Thus, for different values of α , it is possible to explore

the different analytical cases reported in Sec. VII A. However, for the sake of simplicity, we consider explicitly only the results obtained in the framework of the Boltzmann statistics by reporting the following simplified relations for a completely nondegenerate gas:

$$M_{(s)}|_E = n (2s + 1)!! \left(\frac{k_B T}{2} \right)^s \times \left\{ 1 + \frac{\hbar^2}{6m} \frac{s}{k_B T} [\mathcal{Q}^{(2)} + 2(s + 4)\mathcal{Q}^{(3)}] \right\} + O(\hbar^4), \quad s \geq 2, \quad (84)$$

$$M_{(s)|(ij)}|_E = \frac{\hbar^2}{90} \frac{n}{m^2} (2s + 5)!! \left(\frac{k_B T}{2} \right)^s \times \left\{ \mathcal{Q}_{(ij)}^{(4)} + (2s + 7) \mathcal{Q}_{(ij)}^{(5)} \right\} + O(\hbar^4), \quad s \geq 0, \quad (85)$$

$$M_{(s)|i}|_E = 0 + O(\hbar^4), \quad M_{(s)|(i_1 i_2 \dots i_r)}|_E = 0 + O(\hbar^4) \quad (86)$$

with $s \geq 0$ and $r \geq 3$,

where $\{Q^{(2)}, Q^{(3)}, Q_{(ij)}^{(4)}, Q_{(ij)}^{(5)}\}$ expressed by means of the relations (A91) and (A92) in the Appendix.

Also in this case, by using the relations (65)–(67), two degrees of freedom for the remaining system are lost. Indeed, by considering the scalar moments (84) with $s = 0, 1$, we reobtain the relations for the density n and for the quantum pressure (65)₂. Analogously, if we consider the *density-gradient approximation*, then the moments $\{M_{(s)}|_E, M_{(s)|(ij)}|_E\}$ are found to take a simplified form.

2. Equilibrium closure relations

The constitutive relations for the balance equations (A19) and (A20) are represented by the central moments of higher order H_A expressed in Eq. (A24) of the Appendix. Accordingly, to calculate the equilibrium part $H_A|_E$ we can use Eqs. (81)–(83) [or equivalently Eqs. (84)–(86) for a Boltzmann gas]. In particular, for the scalar moments we obtain $M_{(\mathcal{N}+1)}|_E$ from Eq. (81) evaluated for $s = \mathcal{N} + 1$.

VIII. LAGRANGE MULTIPLIERS AND CLOSURE RELATIONS IN NONEQUILIBRIUM CONDITIONS

By inserting the quasi-Moyal approximation (52) into the moments (45) we determine the analytic expression of Lagrange multipliers in nonequilibrium conditions. Conse-

quently, by means of Eq. (26)₂, the constitutive functions (A24) are also obtained in nonequilibrium conditions up to the first quantum correction with respect to the classic expressions.

A. Lagrange multipliers and closure relations for the Fermi and Bose gases

To obtain the nonequilibrium part of the Lagrange multipliers Λ_A all the scalar moments $M_{(s)}$ are separated into the equilibrium and nonequilibrium parts through the relationship $\Delta_{(s)} = M_{(s)} - M_{(s)}|_E$, with $\Delta_{(0)} = \Delta_{(1)} = 0$. Thus, by considering only an arbitrary set of scalar and vectorial moments we find

$$\begin{aligned} \Delta_{(s)} + O(\hbar^4) &= \int d^3 p \tilde{\varepsilon}^s \mathcal{F}_W|_{NE}, \\ M_{(s)|i} + O(\hbar^4) &= \int d^3 p \tilde{\varepsilon}^s \tilde{u}_i \mathcal{F}_W|_{NE}, \end{aligned} \quad (87)$$

where the moments $\{\Delta_{(s)}, M_{(s)|i}\}$ are evaluated up to the first quantum correction. Following this procedure, we obtain a linear system in the nonequilibrium variables $\{\Lambda_{(l)}, \Lambda_{(l)|k}\}$. This system can be solved analytically, and, as reported in the Appendix, the expression of the Lagrange multipliers is determined explicitly by means of relations (A85)–(A87).

From the knowledge of the nonequilibrium Lagrange multipliers and by introducing the expansion (52) in the integrals (26)₂, we obtain the nonequilibrium parts of the constitutive relations (A24). Accordingly, for the scalar moments we find

$$M_{(\mathcal{N}+1)}|_{NE} = \sum_{s=2}^{\mathcal{N}} \left\{ \zeta_{(\mathcal{N}+1)s} + \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[\sum_{p=1}^3 \zeta_{(\mathcal{N}+1)s}^{(1,p)} Q^{(1,p)} + \sum_{q=1}^2 \zeta_{(\mathcal{N}+1)s}^{(2,q)} Q^{(2,q)} \right] \right\} (k_B T)^{\mathcal{N}+1-s} \Delta_{(s)} + O(\hbar^4), \quad (88)$$

with $\mathcal{N} \geq 2$.

For the tensorial moments of second order we obtain

$$M_{(s)|(ij)}|_{NE} = \frac{\hbar^2}{18} \frac{1}{m^2} \left\{ \left[\sum_{r=2}^{\mathcal{N}} \xi_{sr}^{(1,4)} \Delta_{(r)} \right] Q_{(ij)}^{(1,4)} + \left[\sum_{r=2}^{\mathcal{N}} \xi_{sr}^{(2,4)} \Delta_{(r)} \right] Q_{(ij)}^{(2,4)} + \left[\sum_{r=2}^{\mathcal{N}} \xi_{sr}^{(1,5)} \Delta_{(r)} \right] Q_{(ij)}^{(1,5)} \right\} + O(\hbar^4), \quad (89)$$

with $s = 0, \dots, \mathcal{N}$ and $\mathcal{N} \geq 2$.

Analogously, for the tensorial moments of third order we have only the nonequilibrium parts:

$$M_{(s)|(ijk)}|_{NE} = \frac{\hbar^2}{14} \frac{1}{m^2} \left\{ \sum_{r=1}^{\mathcal{N}} \Phi_{sr}^{(1,4)} M_{(r)|(i} Q_{(jk)}^{(1,4)} + \sum_{r=1}^{\mathcal{N}} \Phi_{sr}^{(2,4)} M_{(r)|(i} Q_{(jk)}^{(2,4)} + \sum_{r=1}^{\mathcal{N}} \Phi_{sr}^{(1,5)} M_{(r)|(i} Q_{(jk)}^{(1,5)} \right\} + O(\hbar^4), \quad (90)$$

obtained for $s = 0, \dots, \mathcal{N}$ and $\mathcal{N} \geq 1$.

All moments of higher tensorial order vanish, where

$$M_{(s)|(i_1 i_2 \dots i_r)} = 0 + O(\hbar^4), \quad \text{for } s = 0, \dots, \mathcal{N}, \quad \text{and } r \geq 4, \quad (91)$$

where all the coefficients $\{\zeta_{(\mathcal{N}+1)s}^{(i,j)}, \xi_{(\mathcal{N}+1)s}^{(p,q)}, \xi_{sr}^{(p,q)}, \Phi_{sr}^{(p,q)}\}$ that are present in the above relations are functions explicitly determined through the relations (A88) and (A89) in the Appendix.

B. Boltzmann statistic as limit for $\alpha \gg 1$

We note that the previous relations are valid for various degeneracy levels of Fermi and/or Bose gases, and, for different α values, we can explore all cases explained in Sec. VII A. For the sake of simplicity, here we analyze explicitly only the results obtained for a Boltzmann gas. In this case, $\alpha \gg 1$, we determine explicitly the Lagrange multipliers $\{\Lambda_{(l)}, \Lambda_{(l)k}\}$ as reported in Eqs. (A99) and (A100) of the Appendix. Analogously, by using the relations (88)–(91) and (A88) and (A89) for $\alpha \gg 1$, all constitutive functions can be estimated under nondegenerate conditions. Thus, for the scalar moments in nonequilibrium conditions, we find for $\mathcal{N} \geq 2$:

$$M_{(\mathcal{N}+1)|NE} = \sum_{s=2}^{\mathcal{N}} \left\{ \chi_{(\mathcal{N}+1)s} + \frac{\hbar^2}{12m} \frac{1}{k_B T} \sum_{j=2}^3 [\chi_{(\mathcal{N}+1)s}^{(j)} \mathcal{Q}^{(j)}] \right\} (k_B T)^{\mathcal{N}+1-s} \Delta_{(s)} + O(\hbar^4). \quad (92)$$

For the tensorial moments of second order we find, for $s = 0, \dots, \mathcal{N}$ and $\mathcal{N} \geq 2$:

$$M_{(s)|(ij)|NE} = \frac{\hbar^2}{18} \frac{1}{m^2} \left\{ \left[\sum_{r=2}^{\mathcal{N}} \xi_{sr}^{(4)} \Delta_{(r)} \right] \mathcal{Q}_{(ij)}^{(4)} + \left[\sum_{r=2}^{\mathcal{N}} \xi_{sr}^{(5)} \Delta_{(r)} \right] \mathcal{Q}_{(ij)}^{(5)} \right\} + O(\hbar^4). \quad (93)$$

Analogously, for the tensorial moments of third order, we obtain for $s = 0, \dots, \mathcal{N}$ and $\mathcal{N} \geq 1$:

$$M_{(s)|(ijk)|NE} = \frac{\hbar^2}{14} \frac{1}{m^2} \left\{ \sum_{r=1}^{\mathcal{N}} \Phi_{sr}^{(4)} M_{(r)|(i} \mathcal{Q}_{(jk)}^{(4)} + \sum_{r=1}^{\mathcal{N}} \Phi_{sr}^{(5)} M_{(r)|(i} \mathcal{Q}_{(jk)}^{(5)} \right\} + O(\hbar^4). \quad (94)$$

Finally, all moments of higher tensorial order vanish, being

$$M_{(s)|(i_1 i_2 \dots i_r)} = 0 + O(\hbar^4), \quad \text{for } s = 0, \dots, \mathcal{N}, \quad \text{and } r \geq 4, \quad (95)$$

where all the coefficients of previous relations $\{\chi_{(\mathcal{N}+1)s}, \chi_{(\mathcal{N}+1)s}^{(j)}, \xi_{sr}^{(p)}, \Phi_{sr}^{(p)}\}$ are known functions determined explicitly by means of Eqs. (A93)–(A96), (A101), and (A102) in the Appendix.

1. Simplified model for the density-gradient approximation

We conclude this section by assuming that the nonlocal effects are imputable only to the spatial derivatives of density n . Thus, summarizing the previous results, we obtain the differential constraints (65) [with $Q_B^l \approx Q_B$ and $Q_C^l \approx -(\hbar^2/36m) \Delta \ln n$] for the chemical potential and pressure and, analogously, the following simplified closure relations in both equilibrium and nonequilibrium conditions:

$$\begin{aligned} M_{(\mathcal{N}+1)|E} &= \frac{(2\mathcal{N}+3)!!}{2^{\mathcal{N}+1}} n (k_B T)^{\mathcal{N}+1} \left\{ 1 - \frac{\hbar^2}{36m} \frac{(\mathcal{N}+1)}{k_B T} \frac{\partial^2 \ln n}{\partial x_k \partial x_k} \right\} + O(\hbar^4), \quad \mathcal{N} \geq 1, \\ M_{(\mathcal{N}+1)|NE} &= \sum_{s=2}^{\mathcal{N}} \left\{ \chi_{(\mathcal{N}+1)s} - \frac{\hbar^2}{72m} \frac{\chi_{(\mathcal{N}+1)s}^{(2)}}{k_B T} \frac{\partial^2 \ln n}{\partial x_k \partial x_k} \right\} (k_B T)^{\mathcal{N}+1-s} \Delta_{(s)} + O(\hbar^4), \quad \mathcal{N} \geq 2, \\ M_{(s)|(ij)|E} &= -\frac{\hbar^2}{180} \frac{(2s+5)!!}{2^s} \frac{n}{m^2} (k_B T)^s \frac{\partial^2 \ln n}{\partial x_{(i} \partial x_{j)}} + O(\hbar^4), \quad \mathcal{N} \geq 0, \\ M_{(s)|(ij)|NE} &= -\frac{\hbar^2}{36} \frac{1}{m^2} \left[\sum_{r=2}^{\mathcal{N}} \xi_{sr}^{(4)} \Delta_{(r)} \right] \frac{\partial^2 \ln n}{\partial x_{(i} \partial x_{j)}} + O(\hbar^4), \quad \mathcal{N} \geq 2, \\ M_{(s)|(ijk)|NE} &= -\frac{\hbar^2}{28} \frac{1}{m^2} \sum_{r=1}^{\mathcal{N}} \Phi_{sr}^{(4)} M_{(r)|(i} \frac{\partial^2 \ln n}{\partial x_{(j} \partial x_{k)}} + O(\hbar^4), \quad \mathcal{N} \geq 1, \end{aligned}$$

with $s = 0, \dots, \mathcal{N}$ and $\{\chi_{(\mathcal{N}+1)s}, \chi_{(\mathcal{N}+1)s}^{(2)}, \xi_{sr}^{(4)}, \Phi_{sr}^{(4)}\}$ expressed by (A101) and (A102) in the Appendix.

IX. EXAMPLES AND APPLICATIONS FOR SOME RELEVANT QHD SYSTEM

In the previous sections a complete set of QHD system, to all orders of \hbar , has been constructed. To this purpose, an arbitrary number of scalar and vectorial moments of the Wigner function has been considered as relevant variables, and, by using a QMEP formulation, both the Lagrange multipliers and the closure relations have been determined, up to the first-order quantum approximation, in the algebraic forms (62)–(64), (A85)–(A87), (81)–(83), (88)–(91), (A70)–(A77), (A79)–(A82), and (A88)–(A89). Accordingly, quantum contributions have been determined in powers of \hbar^2 , and, by generalizing the results known in the literature, all the nonlocal effects have been expressed in terms of the spatial derivatives of both the density n and temperature T for the Fermi and/or Bose gases.

In this section we analyze some examples of closed QHD systems, by determining explicitly the constitutive relations, for the correspondent set of equations, up to the first-order quantum correction.

A. Closed QHD system for $\mathcal{N} = 0$

For $\mathcal{N} = 0$ we recover the usual quantum drift-diffusion system (A22) and (A23) for the numerical density n and for the velocity v_i , where it is necessary to assume that the effective temperature is constant (i.e., $T = T_0$) and, consequently, that all nonlocal effects are imputable only to the spatial derivatives of density n . Thus, we find $\beta = (k_B T_0)^{-1}$, while α and P are given by means of the *differential constraints* (63) and (64) evaluated, up to the first-order quantum correction, with $T = T_0$. In this case, for the closure relations we reobtain the results of Ref. [6], being

$$\frac{\partial M_{(0)ik}}{\partial x_k} = \frac{1}{m} \left\{ \frac{\partial P^{(c)}}{\partial x_i} + n \frac{\partial \mu^{(q)}}{\partial x_i} \right\} + O(\hbar^4), \quad (96)$$

where $P^{(c)}$ and $\mu^{(q)}$ represent, respectively, the classical and the quantum parts of the pressure and chemical potential, which can be evaluated explicitly for different regimes of Fermi and/or Bose gases (see Sec. III A of Ref. [6]).

B. Closed QHD system for $\mathcal{N} = 1$

For $\mathcal{N} = 1$ we consider the set of moments $\{n, v_i, P, q_i\}$ where $P = 2/3 M_{(1)}$ and $q_i = M_{(1)i}$ are, respectively, the *pressure* and the *heat flux density*. Thus, by considering Eqs. (A19) and (A20) we obtain the explicit exact QHD system:

$$\frac{\partial n}{\partial t} + \frac{\partial n v_k}{\partial x_k} = 0, \quad (97)$$

$$\frac{\partial v_i}{\partial t} + v_k \frac{\partial v_i}{\partial x_k} + \frac{1}{n} \frac{\partial}{\partial x_k} \left\{ M_{(0)|(ik)} + \frac{P}{m} \delta_{ik} \right\} + \frac{1}{m} \frac{\partial V_{\text{eff}}}{\partial x_i} = 0, \quad (98)$$

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial x_k} \left\{ P v_k + \frac{2}{3} q_k \right\} + \frac{2}{3} P \frac{\partial v_k}{\partial x_k} + \frac{2}{3} m M_{(0)|(ijk)} \frac{\partial v_i}{\partial x_k} = 0, \quad (99)$$

$$\begin{aligned} \frac{\partial q_i}{\partial t} + \frac{\partial}{\partial x_k} \left\{ q_i v_k + M_{(1)|(ik)} + \frac{2}{3} \frac{1}{m} M_{(2)} \delta_{ik} \right\} + m M_{(0)|(ijk)} \frac{\partial v_j}{\partial x_k} + \frac{2}{5} q_i \frac{\partial v_k}{\partial x_k} + \frac{2}{5} q_k \frac{\partial v_i}{\partial x_k} + \frac{7}{5} q_k \frac{\partial v_i}{\partial x_k} \\ - \frac{5}{2} \frac{P}{n} \frac{\partial}{\partial x_k} \left\{ M_{(0)|(ik)} + \frac{P}{m} \delta_{ik} \right\} - \frac{m}{n} M_{(0)|(ij)} \frac{\partial}{\partial x_k} \left\{ M_{(0)|(jk)} + \frac{P}{m} \delta_{jk} \right\} = \frac{\hbar^2}{8m^2} n \frac{\partial^3 V_{\text{eff}}}{\partial x_k^2 \partial x_i}, \end{aligned} \quad (100)$$

with the quantities $H_A = \{M_{(0)|(ik)}, M_{(1)|(ik)}, M_{(2)}, M_{(0)|(ijk)}\}$ as constitutive relations.

In this case we have an effective local and instantaneous temperature $T(\mathbf{r}, t)$, and, in general, the nonlocal effects are imputable to the spatial derivatives of both density and temperature. Accordingly, it is $\beta(\mathbf{r}, t) = [k_B T(\mathbf{r}, t)]^{-1}$ while the system (97)–(100), must be supplemented by the general differential constraints (63) and (64) for α and P .

Analogously, we determine the quantum nonequilibrium Lagrange multipliers by evaluating explicitly the relations (A85)–(A87) for $\mathcal{N} = 1$. Finally, if we know the Lagrange multipliers, then we obtain the Wigner functions up to the first-order quantum correction, and consequently, through the relations (81)–(83), (88)–(91), (A88) and (A89), the explicit closure relations:

$$M_{(0)|(ik)}|_E = -\frac{1}{12} \frac{\hbar^2}{m^2} n \left\{ \frac{I_0^\pm}{I_2^\pm} \mathcal{Q}_{(ik)}^{(1,4)} - 2 \mathcal{Q}_{(ik)}^{(2,4)} + 14 \mathcal{Q}_{(ik)}^{(1,5)} \right\} + O(\hbar^4), \quad (101)$$

$$M_{(1)|(ik)}|_E = -\frac{7}{36} \frac{\hbar^2}{m^2} n k_B T \left\{ 3 \mathcal{Q}_{(ik)}^{(1,4)} - 2 \frac{I_4^\pm}{I_2^\pm} \mathcal{Q}_{(ik)}^{(2,4)} + 18 \frac{I_4^\pm}{I_2^\pm} \mathcal{Q}_{(ik)}^{(1,5)} \right\} + O(\hbar^4), \quad (102)$$

$$M_{(2)}|_E = n \frac{I_6^\pm}{I_2^\pm} (k_B T)^2 \left\{ 1 + \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[\sum_{p=1}^3 \zeta_{1p}^{(2)} \mathcal{Q}^{(1,p)} + \sum_{q=1}^2 \zeta_{2q}^{(2)} \mathcal{Q}^{(2,q)} \right] \right\} + O(\hbar^4), \quad (103)$$

$$M_{(0)|(ijk)}|_{NE} = \frac{3}{4} \frac{\hbar^2}{m^2} \frac{1}{k_B T} \left\{ \tilde{\Phi}^{(1,4)} q_{(i)} \mathcal{Q}_{(jk)}^{(1,4)} + \tilde{\Phi}^{(2,4)} q_{(i)} \mathcal{Q}_{(jk)}^{(2,4)} + \tilde{\Phi}^{(1,5)} q_{(i)} \mathcal{Q}_{(jk)}^{(1,5)} \right\} + O(\hbar^4), \quad (104)$$

where all the coefficients are given, in terms of integral functions $I_n^\pm(\alpha)$, in the form

$$\tilde{\Phi}^{(1,4)} = \frac{27(I_2^\pm)^2 - 5 I_0^\pm I_4^\pm}{25(I_4^\pm)^2 - 21 I_2^\pm I_6^\pm}, \quad \tilde{\Phi}^{(2,4)} = -\frac{8 I_2^\pm I_4^\pm}{25(I_4^\pm)^2 - 21 I_2^\pm I_6^\pm}, \quad \tilde{\Phi}^{(1,5)} = -\frac{27}{2} \tilde{\Phi}^{(2,4)},$$

$$\zeta_{11}^{(2)} = \frac{3}{8} \left[\frac{I_{-4}^\pm}{I_2^\pm} - 5 \frac{I_0^\pm}{I_6^\pm} \right], \quad \zeta_{12}^{(2)} = -\frac{3}{4} \left[\frac{I_{-2}^\pm}{I_2^\pm} + 35 \frac{I_2^\pm}{I_6^\pm} \right], \quad \zeta_{13}^{(2)} = \frac{15}{2} \left[\frac{I_0^\pm}{I_2^\pm} - 21 \frac{I_4^\pm}{I_6^\pm} \right],$$

$$\zeta_{21}^{(2)} = \frac{1}{4} \left[15 \frac{I_2^\pm}{I_6^\pm} + \frac{I_{-2}^\pm}{I_2^\pm} \right], \quad \zeta_{22}^{(2)} = \frac{1}{2} \left[35 \frac{I_4^\pm}{I_6^\pm} - 3 \frac{I_0^\pm}{I_2^\pm} \right],$$

while the nonlocal effects are expressed by terms $\{\mathcal{Q}^{(q,p)}, \mathcal{Q}_{(ik)}^{(q,p)}\}$ in Eqs. (A70)–(A77).

As a simplified approximation, if we consider the *density-gradient approximation*, then we can neglect all spatial derivatives of temperature in Eqs. (101)–(104). Thus, we find $\mathcal{Q}^{(1,3)} = \mathcal{Q}^{(2,2)} = \mathcal{Q}_{(ik)}^{(1,5)} = \mathcal{Q}_{(ik)}^{(2,4)} \approx 0$, while the remaining terms $\{\mathcal{Q}^{(1,1)}, \mathcal{Q}^{(1,2)}, \mathcal{Q}^{(2,1)}, \mathcal{Q}_{(ik)}^{(1,4)}\}$ can be expressed by using Eqs. (A78), and we reobtain, as particular case, the simplified closure relations reported in Sec. III_B of Ref. [6].

1. Boltzmann statistics

Under nondegenerate conditions ($\alpha \gg 1$) both the Fermi and Bose statistics tend to Boltzmann statistic. In particular we obtain the quantum state equation and the quantum chemical potential by (65)–(67), while, using the relations (84)–(86), (92)–(94), and (A102) for $\mathcal{N} = 1$, the constitutive functions are expressed in the form

$$M_{(0)|(ik)}|_E = \frac{1}{6} \frac{\hbar^2}{m^2} n \{ \mathcal{Q}_{(ik)}^{(4)} + 7 \mathcal{Q}_{(ik)}^{(5)} \} + O(\hbar^4), \quad (105)$$

$$M_{(1)|(ik)}|_E = \frac{7}{12} \frac{\hbar^2}{m^2} n k_B T \{ \mathcal{Q}_{(ik)}^{(4)} + 9 \mathcal{Q}_{(ik)}^{(5)} \} + O(\hbar^4), \quad (106)$$

$$M_{(2)}|_E = \frac{15}{4} n (k_B T)^2 \left\{ 1 + \frac{\hbar^2}{3m} \frac{1}{k_B T} [\mathcal{Q}^{(2)} + 12 \mathcal{Q}^{(3)}] \right\} + O(\hbar^4), \quad (107)$$

$$M_{(0)|(ijk)}|_{NE} = \frac{1}{5} \frac{\hbar^2}{m^2} \frac{1}{k_B T} \{ 2 q_i \mathcal{Q}_{(ijk)}^{(4)} + 27 q_i \mathcal{Q}_{(ijk)}^{(5)} \} + O(\hbar^4), \quad (108)$$

with the nonlocal terms $\{\mathcal{Q}^{(j)}, \mathcal{Q}_{(ik)}^{(p)}\}$ given by means of relations (A91) and (A92).

Also in this case, by considering the *density-gradient approximation*, we can neglect all spatial derivatives of temperature in Eqs. (105)–(108), and we reobtain, as particular case, the simplified relations reported in Ref. [6] for a quantum Boltzmann gas.

C. Closed QHD system for $\mathcal{N} = 2$

For $\mathcal{N} = 2$ we consider the exact QHD system in Eqs. (A19) and (A20) for the macroscopic variables $\{n, v_i, P, q_i, M_{(2)}, M_{(2)|i}\}$ where, by decomposing the scalar moments $M_{(2)} = M_{(2)}|_E + \Delta_{(2)}$, the equilibrium part $M_{(2)}|_E$ becomes a new differential constraint for the system, while $\Delta_{(2)}$ represents the new nonequilibrium scalar field variable.

Accordingly, we obtain the previous QHD system (97)–(100) for the moments $\{n, v_i, P, q_i\}$ plus the following set of exact quantum balance equations for the variables $\{M_{(2)}, M_{(2)|i}\}$:

$$\frac{\partial M_{(2)}}{\partial t} + \frac{\partial}{\partial x_k} \{ M_{(2)} v_k + M_{(2)|k} \} + \frac{4}{3} M_{(2)} \frac{\partial v_k}{\partial x_k} + 2m M_{(1)|(ik)} \frac{\partial v_i}{\partial x_k} - 2 \frac{m}{n} q_i \frac{\partial}{\partial x_k} \left\{ M_{(0)|(ik)} + \frac{P}{m} \delta_{ik} \right\} = 0, \quad (109)$$

$$\begin{aligned} & \frac{\partial M_{(2)|i}}{\partial t} + \frac{\partial}{\partial x_k} \left\{ M_{(2)|i} v_k + M_{(2)|(ik)} + \frac{2}{3} \frac{1}{m} M_{(3)} \delta_{ik} \right\} + 2m M_{(1)|(ijk)} \frac{\partial v_j}{\partial x_k} + \frac{4}{5} M_{(2)|i} \frac{\partial v_k}{\partial x_k} + \frac{4}{5} M_{(2)|k} \frac{\partial v_k}{\partial x_i} \\ & + \frac{9}{5} M_{(2)|k} \frac{\partial v_i}{\partial x_k} - \frac{7}{3} \frac{M_{(2)}}{n} \frac{\partial}{\partial x_k} \left\{ M_{(0)|(ik)} + \frac{P}{m} \delta_{ik} \right\} - 2 \frac{m}{n} M_{(1)|(ij)} \frac{\partial}{\partial x_k} \left\{ M_{(0)|(jk)} + \frac{P}{m} \delta_{jk} \right\} \\ & = \frac{\hbar^2}{4m} \left\{ \frac{\partial^3 V_{\text{eff}}}{\partial x_k^2 \partial x_r} M_{(0)|(ri)} + \frac{\partial^3 V_{\text{eff}}}{\partial x_k \partial x_r \partial x_i} M_{(0)|(kr)} + \frac{7}{2} \frac{P}{m} \frac{\partial^3 V_{\text{eff}}}{\partial x_k^2 \partial x_i} \right\} - \frac{\hbar^4}{64m^3} n \frac{\partial^5 V_{\text{eff}}}{\partial x_k^2 \partial x_r^2 \partial x_i}, \end{aligned} \quad (110)$$

where the quantities $H_A = \{M_{(0)|(ik)}, M_{(1)|(ik)}, M_{(2)|(ik)}, M_{(3)}, M_{(0)|(ijk)}, M_{(1)|(ijk)}\}$ represent the set of constitutive relations for the system.

In this case, the exact QHD equations (97)–(100), (109) and (110) must be supplemented by the differential constraints in Eqs. (63), (64), and (103) to determine, respectively, α , P , and $M_{(2)}|_E$ up to the first-order quantum correction. The equilibrium parts of the constitutive functions $H_A|_E = \{M_{(0)|(ik)}|_E, M_{(1)|(ik)}|_E, M_{(2)|(ik)}|_E, M_{(3)}|_E\}$ are given by (101) and (102) and by means of equations

$$M_{(2)|(ik)}|_E = -\frac{7}{20} \frac{\hbar^2}{m^2} n (k_B T)^2 \left\{ 5 \frac{I_4^\pm}{I_2^\pm} \mathcal{Q}_{(ik)}^{(1,4)} - 2 \frac{I_6^\pm}{I_2^\pm} \mathcal{Q}_{(ik)}^{(2,4)} + 22 \frac{I_6^\pm}{I_2^\pm} \mathcal{Q}_{(ik)}^{(1,5)} \right\} + O(\hbar^4), \quad (111)$$

$$M_{(3)}|_E = n \frac{I_8^\pm}{I_2^\pm} (k_B T)^3 \left\{ 1 + \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[\sum_{p=1}^3 \zeta_{1p}^{(3)} \mathcal{Q}^{(1,p)} + \sum_{q=1}^2 \zeta_{2q}^{(3)} \mathcal{Q}^{(2,q)} \right] \right\} + O(\hbar^4), \quad (112)$$

where

$$\begin{aligned}\zeta_{11}^{(3)} &= \frac{3}{8} \left[\frac{I_{-4}^{\pm}}{I_2^{\pm}} - 35 \frac{I_2^{\pm}}{I_8^{\pm}} \right], & \zeta_{12}^{(3)} &= -\frac{3}{4} \left[\frac{I_{-2}^{\pm}}{I_2^{\pm}} + 105 \frac{I_4^{\pm}}{I_8^{\pm}} \right], & \zeta_{13}^{(3)} &= \frac{3}{2} \left[5 \frac{I_0^{\pm}}{I_2^{\pm}} - 231 \frac{I_6^{\pm}}{I_8^{\pm}} \right], \\ \zeta_{21}^{(3)} &= \frac{1}{4} \left[35 \frac{I_4^{\pm}}{I_8^{\pm}} + \frac{I_{-2}^{\pm}}{I_2^{\pm}} \right], & \zeta_{22}^{(3)} &= \frac{3}{2} \left[21 \frac{I_6^{\pm}}{I_8^{\pm}} - \frac{I_0^{\pm}}{I_2^{\pm}} \right].\end{aligned}$$

Analogously, for $s = 0, 1, 2$ and $r = 0, 1$, the nonequilibrium parts of the constitutive functions H_A are expressed up to the first-order quantum correction in the compact form

$$M_{(s)|(ij)}|_{NE} = \frac{\hbar^2}{18m^2} \{ \xi_{s2}^{(1,4)} \mathcal{Q}_{(ij)}^{(1,4)} + \xi_{s2}^{(2,4)} \mathcal{Q}_{(ij)}^{(2,4)} + \xi_{s2}^{(1,5)} \mathcal{Q}_{(ij)}^{(1,5)} \} \Delta_{(2)} + O(\hbar^4), \quad (113)$$

$$M_{(3)}|_{NE} = \left\{ \zeta_{32} (k_B T) + \frac{\hbar^2}{12m} \left[\sum_{p=1}^3 \zeta_{32}^{(1,p)} \mathcal{Q}^{(1,p)} + \sum_{q=1}^2 \zeta_{32}^{(2,q)} \mathcal{Q}^{(2,q)} \right] \right\} \Delta_{(2)} + O(\hbar^4), \quad (114)$$

$$\begin{aligned}M_{(r)|(ijk)}|_{NE} &= \frac{\hbar^2}{14m^2} \{ \Phi_{r1}^{(1,4)} q_i \mathcal{Q}_{(jk)}^{(1,4)} + \Phi_{r1}^{(2,4)} q_i \mathcal{Q}_{(jk)}^{(2,4)} + \Phi_{r1}^{(1,5)} q_i \mathcal{Q}_{(jk)}^{(1,5)} \\ &+ \Phi_{r2}^{(1,4)} M_{(2)|(i} \mathcal{Q}_{(jk)}^{(1,4)} + \Phi_{r2}^{(2,4)} M_{(2)|(i} \mathcal{Q}_{(jk)}^{(2,4)} + \Phi_{r2}^{(1,5)} M_{(2)|(i} \mathcal{Q}_{(jk)}^{(1,5)} \} + O(\hbar^4),\end{aligned} \quad (115)$$

where all the coefficients $\{ \xi_{s2}^{(l,n)}, \zeta_{32}, \zeta_{32}^{(1,p)}, \zeta_{32}^{(2,q)}, \Phi_{rq}^{(l,n)} \}$ can be obtained explicitly through the algebraic relations (A88) and (A89) evaluated for $\mathcal{N} = 2$, while the nonlocal terms $\{ \mathcal{Q}^{(q,p)}, \mathcal{Q}_{(jk)}^{(l,n)} \}$ are given in Eqs. (A70)–(A77).

Finally, if we consider the *density-gradient approximation*, then we can neglect the spatial derivatives of temperature in all previous relations, and using Eqs. (A78), it is possible to determine the simplified expressions for the first-order quantum correction terms.

I. Boltzmann statistics

In the framework of Boltzmann statistics (i.e., for $\alpha \gg 1$), the system (97)–(100) plus Eqs. (109) and (110), for the variables $\{ n, v_i, P, q_i, \Delta_{(2)}, M_{(2)|i} \}$, are supplemented by Eqs. (65)–(67) and (107), respectively, for μ, P and $M_{(2)}|_E$. Therefore, in equilibrium conditions, for the constitutive functions we obtain $M_{(0)|(ik)}|_E$ and $M_{(1)|(ik)}|_E$ by Eqs. (105) and (106) and $\{ M_{(2)|(ik)}|_E, M_{(3)}|_E \}$ by means of relations

$$M_{(2)|(ik)}|_E = \frac{21}{8} \frac{\hbar^2}{m^2} n (k_B T)^2 \{ \mathcal{Q}_{(ik)}^{(4)} + 11 \mathcal{Q}_{(ik)}^{(5)} \} + O(\hbar^4), \quad (116)$$

$$M_{(3)}|_E = \frac{105}{8} n (k_B T)^3 \left\{ 1 + \frac{\hbar^2}{2m} \frac{1}{k_B T} [\mathcal{Q}^{(2)} + 14 \mathcal{Q}^{(3)}] \right\} + O(\hbar^4). \quad (117)$$

Analogously, in nonequilibrium conditions, for the constitutive functions we obtain

$$M_{(0)|(ik)}|_{NE} = \frac{2}{45} \frac{\hbar^2}{m^2} \frac{1}{(k_B T)^2} \{ \mathcal{Q}_{(ik)}^{(4)} + 21 \mathcal{Q}_{(ik)}^{(5)} \} \Delta_{(2)} + O(\hbar^4), \quad (118)$$

$$M_{(1)|(ik)}|_{NE} = \frac{7}{15} \frac{\hbar^2}{m^2} \frac{1}{k_B T} \{ \mathcal{Q}_{(ik)}^{(4)} + 18 \mathcal{Q}_{(ik)}^{(5)} \} \Delta_{(2)} + O(\hbar^4), \quad (119)$$

$$M_{(2)|(ik)}|_{NE} = \frac{7}{5} \frac{\hbar^2}{m^2} \{ 3 \mathcal{Q}_{(ik)}^{(4)} + 55 \mathcal{Q}_{(ik)}^{(5)} \} \Delta_{(2)} + O(\hbar^4), \quad (120)$$

$$M_{(3)}|_{NE} = \frac{21}{2} k_B T \left\{ 1 + \frac{\hbar^2}{6m} \frac{1}{k_B T} [\mathcal{Q}^{(2)} + 26 \mathcal{Q}^{(3)}] \right\} \Delta_{(2)} + O(\hbar^4), \quad (121)$$

$$M_{(0)|(ijk)}|_{NE} = -\frac{1}{35} \frac{\hbar^2}{m^2} \frac{1}{(k_B T)^2} \{ 189 k_B T q_i \mathcal{Q}_{(jk)}^{(5)} - 2 [M_{(2)|(i} \mathcal{Q}_{(jk)}^{(4)} + 27 M_{(2)|(i} \mathcal{Q}_{(jk)}^{(5)}] \} + O(\hbar^4), \quad (122)$$

$$M_{(1)|(ijk)}|_{NE} = -\frac{9}{70} \frac{\hbar^2}{m^2} \frac{1}{k_B T} \{ 7 k_B T [3 q_i \mathcal{Q}_{(jk)}^{(4)} + 88 q_i \mathcal{Q}_{(jk)}^{(5)}] - 6 [M_{(2)|(i} \mathcal{Q}_{(jk)}^{(4)} + 22 M_{(2)|(i} \mathcal{Q}_{(jk)}^{(5)}] \} + O(\hbar^4), \quad (123)$$

with the nonlocal terms $\{ \mathcal{Q}^{(j)}, \mathcal{Q}_{(ik)}^{(p)} \}$ given in Eqs. (A91) and (A92).

Finally, if we assume the *density-gradient approximation*, then we introduce the Bohm quantum potential Q_B , and we obtain for μ , P , and $M_{(2)}|_E$ the simplified explicit quantities

$$\mu = k_B T \ln \left[\frac{n}{2\bar{s} + 1} \left(\frac{2\pi\hbar^2}{mk_B T} \right)^{\frac{3}{2}} \right] + \frac{Q_B}{3} + O(\hbar^4), \quad P = nk_B T - \frac{\hbar^2}{36m} \frac{n}{\partial x_r \partial x_r} + O(\hbar^4), \quad (124)$$

$$M_{(2)}|_E = \frac{15}{4} n (k_B T)^2 \left\{ 1 - \frac{\hbar^2}{18m} \frac{1}{k_B T} \frac{\partial^2 \ln n}{\partial x_r \partial x_r} \right\} + O(\hbar^4). \quad (125)$$

Analogously, for the equilibrium constitutive functions we find the relations

$$M_{(r)|(ij)}|_E = -\frac{\hbar^2}{180} \frac{(2r+5)!!}{2^r} \frac{n}{m^2} (k_B T)^r \frac{\partial^2 \ln n}{\partial x_{(i} \partial x_{j)}} + O(\hbar^4) \quad \text{with } r = 0, 1, 2, \quad (126)$$

$$M_{(3)}|_E = \frac{105}{8} n (k_B T)^3 \left\{ 1 - \frac{\hbar^2}{12m} \frac{1}{k_B T} \frac{\partial^2 \ln n}{\partial x_r \partial x_r} \right\} + O(\hbar^4), \quad (127)$$

while, in nonequilibrium conditions, we obtain the simplified explicit expressions

$$M_{(0)|(ik)}|_{NE} = -\frac{1}{45} \frac{\hbar^2}{m^2} \frac{1}{(k_B T)^2} \frac{\partial^2 \ln n}{\partial x_{(i} \partial x_{k)}} \Delta_{(2)} + O(\hbar^4), \quad (128)$$

$$M_{(1)|(ik)}|_{NE} = -\frac{7}{30} \frac{\hbar^2}{m^2} \frac{1}{k_B T} \frac{\partial^2 \ln n}{\partial x_{(i} \partial x_{k)}} \Delta_{(2)} + O(\hbar^4), \quad (129)$$

$$M_{(2)|(ik)}|_{NE} = -\frac{21}{10} \frac{\hbar^2}{m^2} \frac{\partial^2 \ln n}{\partial x_{(i} \partial x_{k)}} \Delta_{(2)} + O(\hbar^4), \quad (130)$$

$$M_{(3)}|_{NE} = \frac{21}{2} k_B T \left\{ 1 - \frac{\hbar^2}{36m} \frac{1}{k_B T} \frac{\partial^2 \ln n}{\partial x_r \partial x_r} \right\} \Delta_{(2)} + O(\hbar^4), \quad (131)$$

$$M_{(0)|(ijk)}|_{NE} = -\frac{1}{35} \frac{\hbar^2}{m^2} \frac{1}{(k_B T)^2} M_{(2)|(i} \frac{\partial^2 \ln n}{\partial x_{(j} \partial x_{k)}} + O(\hbar^4), \quad (132)$$

$$M_{(1)|(ijk)}|_{NE} = \frac{27}{140} \frac{\hbar^2}{m^2} \frac{1}{k_B T} \left\{ 7 k_B T q_{(i} \frac{\partial^2 \ln n}{\partial x_{(j} \partial x_{k)}} - 2 M_{(2)|(i} \frac{\partial^2 \ln n}{\partial x_{(j} \partial x_{k)}} \right\} + O(\hbar^4). \quad (133)$$

X. CONCLUSIONS

The quantum maximum entropy principle (QMEP) is here asserted as the fundamental principle of quantum statistical mechanics when it becomes necessary to treat systems in partially specified quantum mechanical states. To this purpose, we have presented a rigorous nonlocal formulation of QMEP by using a quantum entropy that includes indistinguishability for a system of identical particles [6]. Accordingly, we have provided a general framework for the development of quantum hydrodynamic models, which allows a systematic analysis of quantum effects in powers of \hbar^2 to be carried out.

Relevant results reported in the paper are the following:

(i) The development of a proper nonlocal formulation of QMEP, in both thermodynamic equilibrium and nonequilibrium conditions, by determining an explicit functional form in Eq. (34) of the reduced density operator, which requires the consistent introduction of nonlocal quantum Lagrange multipliers within a Moyal expansion, as given in Eqs. (63), (A70)–(A77), (A79)–(A81), and (A85)–(A87).

(ii) The inclusion of statistics effects in the formulation of the QMEP for any degeneracy levels of Fermi and Bose gases.

(iii) The determination of some systematic recursive relations that close rigorously a QHD system for an arbitrary number of scalar and vectorial central moments, in both thermodynamic equilibrium and nonequilibrium conditions. Examples of this procedure are developed explicitly for the first three set of QHD systems.

We stress that quantum transport equations far more general than standard ones, incorporating nonlocal and nonlinear terms, are a demanding issue in current frontiers of technology. The present theory provides an answer to this issue by generalizing most of the results available in the literature since all nonlocal effects are expressed taking into account both the density and temperature high-order spatial derivatives, and obtaining an expansion of the corresponding Lagrange multipliers in terms of powers of the Planck constant, in both equilibrium and nonequilibrium conditions. In particular, when the spatial derivatives of the effective temperature are very large in the regions where the numerical density also varies very quickly, and these regions are comparable with the mean-free path of particles, then nonlocal effects due to the effective temperature gradients cannot be neglected [20]. By contrast, in the *density gradient approximation* all nonlocal effects are imputable only to spatial derivatives of the numerical density, and we recover well-known results for a quantum Boltzmann gas [23,24], for a completely degenerate

Fermi gas [25–27,57] and, more generally, for Fermi and Bose gases [6]. Here QMEP allows one to describe the thermodynamic evolution of a nonequilibrium system in the framework of a nonlocal theory compatibly with the kind of statistics and the uncertainty principle.

We finally remark that the character of some variational principles shows some formal analogies between the apparatus of nonequilibrium thermodynamics and mechanics [58]. To this purpose, all the above results point us to consider the principle of maximum entropy as a fundamental postulate of statistical mechanics in close analogy with the least action principle of mechanics [59].

ACKNOWLEDGMENTS

This research is supported by INDAM, GNFM project Young Researchers (2010) and MIUR-PRIN project Nonlinear Propagation and Stability in Thermodynamical Processes of Continuous Media.

APPENDIX

This appendix collects the mathematical details associated with the formulation of the quantum hydrodynamic models developed in the main text. The objective is to provide the major clues for the reader to reproduce the analytical results presented here within an affordable effort.

1. General relationships

(I) For any couple of analytical functions $V = V(\mathbf{r}, t)$ and $\psi = \psi(\mathbf{r}, \mathbf{p}, t)$, this holds the property

$$\frac{\partial^{2l+1} V}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \int d^3 p \frac{\partial^{2l+1} \mathcal{F}_{\mathcal{W}}}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} \psi = - \frac{\partial^{2l+1} V}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \int d^3 p \frac{\partial^{2l+1} \psi}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} \mathcal{F}_{\mathcal{W}}, \quad (\text{A1})$$

where the Einstein convention is here and henceforth assumed on the saturated indices. For the proof we use the identity

$$\begin{aligned} \frac{\partial^{2l+1} V}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \int d^3 p \frac{\partial^{2l+1} \mathcal{F}_{\mathcal{W}}}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} \psi = & - \frac{\partial^{2l+1} V}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \int d^3 p \frac{\partial^{2l+1} \psi}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} \mathcal{F}_{\mathcal{W}} \\ & + \frac{\partial^{2l+1} V}{\partial x_r \partial x_{k_1} \cdots \partial x_{k_{2l}}} \int d^3 p \frac{\partial}{\partial p_r} \left\{ \sum_{j=0}^{2l} (-1)^j \frac{\partial^{2l-j} \mathcal{F}_{\mathcal{W}}}{\partial p_{k_1} \cdots \partial p_{k_{2l-j}}} \frac{\partial^j \psi}{\partial p_{k_{2l-j+1}} \cdots \partial p_{k_{2l}}} \right\}, \end{aligned}$$

and, with $V = V(\mathbf{r}, t)$, we apply the Gauss theorem in the last term of the above identity. In this case the surface integral should be taken over the momentum shell for $\mathbf{p} \rightarrow \infty$, where it vanishes since the Wigner function and its derivatives $\mathcal{F}_{\mathcal{W}}|_{\mathbf{p} \rightarrow \infty} = \frac{\partial^r \mathcal{F}_{\mathcal{W}}}{\partial p_{k_1} \cdots \partial p_{k_r}}|_{\mathbf{p} \rightarrow \infty} = 0 \quad \forall r > 0$.

(II) We consider two arbitrary operators $\widehat{A}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$ and $\widehat{B}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$ being $A(\mathbf{r}, \mathbf{p})$ and $B(\mathbf{r}, \mathbf{p})$ the corresponding space-phase functions. By using the Moyal formalism [50], the Weyl-Wigner transform of the product of these operators reads

$$\mathcal{W}(\widehat{A} \widehat{B}) = \widehat{A} \star \widehat{B} = \sum_{s=0}^{+\infty} \hbar^s A(\mathbf{r}, \mathbf{p}) \star_s B(\mathbf{r}, \mathbf{p}), \quad (\text{A2})$$

where, for convenience, the general term is expressed in the form

$$A(\mathbf{r}, \mathbf{p}) \star_s B(\mathbf{r}, \mathbf{p}) = \left(\frac{i}{2}\right)^s \frac{1}{s!} \sum_{k=0}^s (-1)^k \frac{s!}{(s-k)! k!} \left[\frac{\partial^{s-k}}{\partial x_{i_1} \cdots \partial x_{i_{s-k}}} \frac{\partial^k A(\mathbf{r}, \mathbf{p})}{\partial p_{j_1} \cdots \partial p_{j_k}} \right] \left[\frac{\partial^k}{\partial x_{j_1} \cdots \partial x_{j_k}} \frac{\partial^{s-k} B(\mathbf{r}, \mathbf{p})}{\partial p_{i_1} \cdots \partial p_{i_{s-k}}} \right], \quad (\text{A3})$$

with the Einstein convention on the saturated indices, where

$$A(\mathbf{r}, \mathbf{p}) \star_s B(\mathbf{r}, \mathbf{p}) = (-1)^s B(\mathbf{r}, \mathbf{p}) \star_s A(\mathbf{r}, \mathbf{p}). \quad (\text{A4})$$

In particular, it is easy to show that, if $[\widehat{A}, \widehat{B}] = 0$, then

$$\mathcal{W}(\widehat{A} \widehat{B}) = \widehat{A} \star \widehat{B} = \sum_{s=0}^{+\infty} \hbar^{2s} A(\mathbf{r}, \mathbf{p}) \star_{2s} B(\mathbf{r}, \mathbf{p}). \quad (\text{A5})$$

(III) By assuming that $A(\mathbf{r}, \mathbf{p})$ is expressed by an expansion in an even power of \hbar as

$$A(\mathbf{r}, \mathbf{p}) = \sum_{r=0}^{\infty} \hbar^{2r} A_{2r}(\mathbf{r}, \mathbf{p}), \quad (\text{A6})$$

it is possible to define the functions

$$H_{2s}^{\pm}(\tau, \mathbf{r}, \mathbf{p}) = \sum \frac{(\pm\tau)^m}{i_1! i_2! \dots i_l!} (A_2)^{i_1} (A_4)^{i_2} \dots (A_{2l})^{i_l} \quad \forall s \geq 0, \quad (\text{A7})$$

where τ is an arbitrary scalar parameter, and \sum indicates summation over all the solutions in non-negative integers of the equations $i_1 + 2i_2 + \dots + li_l = s$ and $i_1 + i_2 + \dots + i_l = m$. Analogously, we can define the recursive functions

$$G_0^{\pm} = 1, \quad \text{and} \quad G_{2s}^{\pm}(\tau, \mathbf{r}, \mathbf{p}) = -\frac{e^{\tau A_0}}{e^{\tau A_0} \pm 1} \sum_{k=0}^{s-1} G_{2k}^{\pm} H_{2(s-k)}^{\pm} \quad \text{for} \quad \forall s \geq 1, \quad (\text{A8})$$

and obtain the following expansions in an even power of \hbar :

$$e^{\tau A(\mathbf{r}, \mathbf{p})} = e^{\tau A_0} \sum_{r=0}^{\infty} \hbar^{2r} H_{2r}^+(\tau, \mathbf{r}, \mathbf{p}), \quad \frac{1}{e^{\tau A(\mathbf{r}, \mathbf{p})} \pm 1} = \frac{1}{e^{\tau A_0} \pm 1} \sum_{r=0}^{\infty} \hbar^{2r} G_{2r}^{\pm}(\tau, \mathbf{r}, \mathbf{p}). \quad (\text{A9})$$

By introducing the integral functions

$$V_{2s}^+(\tau, \mathbf{r}, \mathbf{p}) = \int_0^{\tau} H_{2s}^+(\xi, \mathbf{r}, \mathbf{p}) d\xi, \quad (\text{A10})$$

and a set of *arbitrary functions* $\{L_{2k}\}$ (with k a positive integer), one can verify the following algebraic recurrence relations:

$$\sum_{s=1}^r A_{2s} V_{2(r-s)}^+ = H_{2r}^+, \quad (\text{A11})$$

$$\sum_{s=1}^r L_{2s} H_{2(r+1-s)}^+ = \sum_{m=1}^r A_{2m} \sum_{k=1}^{r+1-m} L_{2k} V_{2(r+1-m-k)}^+, \quad (\text{A12})$$

$$\sum_{s=1}^r L_{2s} H_{2(r-s)}^- = L_{2r} - \sum_{m=1}^{r-1} A_{2m} \sum_{k=1}^{r-m} V_{2(r-m-k)}^+ \sum_{q=1}^k L_{2q} H_{2(k-q)}^-, \quad (\text{A13})$$

$$\sum_{s=1}^r G_{2s}^{\pm} L_{2(r+1-s)} = -\frac{e^{\tau A_0}}{e^{\tau A_0} \pm 1} \sum_{m=1}^r H_{2(r+1-m)}^+ \sum_{k=0}^{m-1} G_{2k}^{\pm} L_{2(m-k)}, \quad (\text{A14})$$

for $\forall r \geq 1$.

2. Full gradient expansion of the Wigner equation

By introducing in Eq. (14) the identity

$$\phi_k e^{-\frac{i}{\hbar} \phi \cdot \mathbf{r}'} = -\frac{\hbar}{i} \frac{\partial e^{-\frac{i}{\hbar} \phi \cdot \mathbf{r}'}}{\partial x'_k}$$

and where $\mathcal{F}_{\mathcal{W}}|_{\mathbf{r} \rightarrow \infty} = 0$, we obtain

$$\frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial t} = -\frac{p_k}{m} \frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial x_k} - \frac{i/\hbar}{(2\pi\hbar)^3} \int d^3\tau e^{-\frac{i}{\hbar} \tau \cdot \mathbf{p}} [V_{\text{eff}}(\mathbf{r} + \tau/2) - V_{\text{eff}}(\mathbf{r} - \tau/2)] \int d^3p' e^{\frac{i}{\hbar} \tau \cdot \mathbf{p}'} \mathcal{F}_{\mathcal{W}}.$$

By expanding the term $V_{\text{eff}}(\mathbf{r} + \tau/2) - V_{\text{eff}}(\mathbf{r} - \tau/2)$ in the McLaurin series around $\tau = 0$, and using the identity

$$\tau_{k_1} \tau_{k_2} \dots \tau_{k_{2l+1}} e^{\frac{i}{\hbar} \tau \cdot \mathbf{p}'} = \left(\frac{\hbar}{i}\right)^{2l+1} \frac{\partial^{2l+1} e^{\frac{i}{\hbar} \tau \cdot \mathbf{p}'}}{\partial p'_{k_1} \partial p'_{k_2} \dots \partial p'_{k_{2l+1}}}, \quad (\text{A15})$$

we obtain

$$\frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial t} + \frac{p_k}{m} \frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial x_k} = -\frac{1}{(2\pi\hbar)^3} \sum_{l=0}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \int d^3\tau e^{-\frac{i}{\hbar} \tau \cdot \mathbf{p}} \left\{ \frac{\partial^{2l+1} V_{\text{eff}}}{\partial x_{k_1} \dots \partial x_{k_{2l+1}}} \int d^3p' \frac{\partial^{2l+1} e^{\frac{i}{\hbar} \tau \cdot \mathbf{p}'}}{\partial p'_{k_1} \dots \partial p'_{k_{2l+1}}} \mathcal{F}_{\mathcal{W}} \right\}, \quad (\text{A16})$$

where the Einstein k convention is assumed on the saturated indices k_1, \dots, k_{2l+1} .

Finally, by using Eq. (A1) and the Fourier integral theorem, the full expansion of the generalized Wigner equation to all order of \hbar takes the form reported in Eq. (17).

3. Quantum corrections to all orders of \hbar for the hydrodynamic equations

In general, the balance equations are obtained through multiplication of the Wigner equations (17) by an arbitrary function $\psi(\mathbf{r}, \mathbf{p}, t)$ and integration over \mathbf{p} . Accordingly, it is

$$\begin{aligned} & \frac{\partial}{\partial t} \int d^3 p \psi \mathcal{F}_{\mathcal{W}} + \frac{\partial}{\partial x_k} \int d^3 p \psi (\tilde{u}_k + v_k) \mathcal{F}_{\mathcal{W}} - \int d^3 p \left[\frac{\partial \psi}{\partial t} + (\tilde{u}_k + v_k) \frac{\partial \psi}{\partial x_k} \right] \mathcal{F}_{\mathcal{W}} \\ &= - \sum_{l=0}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \frac{\partial^{2l+1} V_{\text{eff}}}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \int d^3 p \frac{\partial^{2l+1} \psi}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} \mathcal{F}_{\mathcal{W}}, \end{aligned} \quad (\text{A17})$$

where the quantity in the right-hand side of Eq. (A17) is obtained by using Eq. (A1). In particular, by considering as set of kinetic fields the quantities $\psi_A = \{\tilde{\varepsilon}^s, \tilde{\varepsilon}^s \tilde{u}_i\}$ we obtain

$$\frac{\partial^{2l+1} \tilde{\varepsilon}^s}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} = 0 \quad \text{if } l \geq s, \quad \frac{\partial^{2l+1} \tilde{\varepsilon}^s \tilde{u}_i}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} = 0 \quad \text{if } l \geq s+1;$$

otherwise

$$\begin{aligned} \frac{\partial^{2l+1} \tilde{\varepsilon}^s}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} &= \sum_{r=q}^l B_{sl}^{(0)r} \tilde{\varepsilon}^{s+r-(2l+1)} \delta_{(k_1 k_2 \cdots k_{2r-1} k_{2r})} \tilde{u}_{k_{2r+1}} \cdots \tilde{u}_{k_{2l+1}}, \quad l \in [0, s-1], \\ \frac{\partial^{2l+1} \tilde{\varepsilon}^s \tilde{u}_i}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} &= \sum_{r=q}^{l+1} B_{sl}^{(1)r} \tilde{\varepsilon}^{s+r-(2l+1)} \delta_{(k_1 k_2 \cdots k_{2r-1} k_{2r})} \tilde{u}_{k_{2r+1}} \cdots \tilde{u}_{k_{2l+2}} \delta_{k_{2l+2} i}, \quad l \in [0, s], \end{aligned}$$

where $q = \max\{0, (2l+1-s)\}$ and

$$B_{sl}^{(p)r} = \frac{s!}{[s+r-(2l+1)]!} \frac{[(2l+1)+p]!}{[2(l-r)+1+p]! (2r)!} \frac{1}{m^r} \quad \text{for } p = 0, 1. \quad (\text{A18})$$

By inserting the above relations in Eq. (A17) and considering the traceless parts of the tensorial moments, we obtain the quantum balance equations for the scalar and vectorial moments $\{M_{(s)}, M_{(s)i}\}$ to all orders of \hbar , with $s = 0, 1, \dots, \mathcal{N}$:

$$\begin{aligned} & \dot{M}_{(s)} + M_{(s)} \frac{\partial v_k}{\partial x_k} + \frac{\partial M_{(s)k}}{\partial x_k} + s m M_{(s-1)ik} \frac{\partial v_i}{\partial x_k} + s m M_{(s-1)i} \left[\dot{v}_i + \frac{1}{m} \frac{\partial V_{\text{eff}}}{\partial x_i} \right] \\ &= - \sum_{l=1}^{s-1} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \sum_{r=q}^l B_{sl}^{(0)r} \left\{ \frac{\partial^{2r}}{\partial x_{\beta_1}^2 \cdots \partial x_{\beta_r}^2} \frac{\partial^{2(l-r)+1} V_{\text{eff}}}{\partial x_{k_1} \cdots \partial x_{k_{2(l-r)+1}}} M_{(s+r-2l-1)|(k_1 \cdots k_{2(l-r)+1})} \right. \\ & \quad \left. + \sum_{j=1}^{l-r} A_{lr}^{(0)j} \frac{\partial^{2(r+j)}}{\partial x_{\beta_1}^2 \cdots \partial x_{\beta_{r+j}}^2} \frac{\partial^{2(l-r-j)+1} V_{\text{eff}}}{\partial x_{k_1} \cdots \partial x_{k_{2(l-r-j)+1}}} M_{(s+r+j-2l-1)|(k_1 \cdots k_{2(l-r-j)+1})} \right\}, \end{aligned} \quad (\text{A19})$$

$$\begin{aligned} & \dot{M}_{(s)i} + M_{(s)i} \frac{\partial v_k}{\partial x_k} + \frac{\partial M_{(s)ik}}{\partial x_k} + s m M_{(s-1)ipk} \frac{\partial v_p}{\partial x_k} + M_{(s)} \left[\dot{v}_i + \frac{1}{m} \frac{\partial V_{\text{eff}}}{\partial x_i} \right] \\ & + M_{(s)k} \frac{\partial v_i}{\partial x_k} + s m M_{(s-1)ik} \left[\dot{v}_k + \frac{1}{m} \frac{\partial V_{\text{eff}}}{\partial x_k} \right] = - \sum_{l=1}^s \frac{(i\hbar/2)^{2l}}{(2l+1)!} \frac{\partial^{2l+1} V_{\text{eff}}}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \\ & \times \sum_{r=q}^{l+1} B_{sl}^{(1)r} \left\{ M_{(s+r-2l-1)|(k_1 \cdots k_{2(l-r)+2})} \delta_{k_{2(l-r)+3} k_{2(l-r)+4}} \cdots \delta_{k_{2l+1} i} \right. \\ & \quad \left. + \sum_{j=1}^{l-r+1} A_{lr}^{(1)j} M_{(s+r+j-2l-1)|(k_1 \cdots k_{2(l-r-j)+2})} \delta_{k_{2(l-r-j)+3} k_{2(l-r-j)+4}} \cdots \delta_{k_{2l+1} i} \right\}, \end{aligned} \quad (\text{A20})$$

where $\{B_{sl}^{(0)r}, B_{sl}^{(1)r}\}$ are expressed by Eq. (A18) and the quantities $\{A_{lr}^{(0)j}, A_{lr}^{(1)j}\}$ by

$$A_{lr}^{(p)j} = \frac{[2(l-r)+1+p]!}{[2(l-r-j)+1+p]!} \frac{[4(l-r-j)+2p+3]!!}{[4(l-r)-2j+2p+3]!! (j)!} \frac{1}{m^j} \quad \text{for } p = 0, 1. \quad (\text{A21})$$

Accordingly, by considering Eqs. (A19) and (A20) for $s = 0$ we find the usual balance equations for the density $n = M_{(0)}$ and velocity v_i :

$$\dot{n} + n \frac{\partial v_k}{\partial x_k} = 0, \quad (\text{A22})$$

$$\dot{v}_i + \frac{1}{n} \frac{\partial M_{(0)ik}}{\partial x_k} + \frac{1}{m} \frac{\partial V_{\text{eff}}}{\partial x_i} = 0, \quad (\text{A23})$$

while the remaining equations (for $s = 1, \dots, \mathcal{N}$) can be expressed by eliminating explicitly all time derivatives \dot{v}_i through Eq. (A23). Thus we obtain all the balance equations rewritten explicitly in the form reported in Ref. [6], and, for $\hbar \rightarrow 0$, we recover the classic form of extended thermodynamics [1,7,60,61].

It should be noted that, by using the complete expansion in Eq. (17), it follows that in each QHD scalar and vectorial equation only a finite number of terms in powers of \hbar^2 remains. Thus, for any fixed number of scalar and vectorial moments (i.e., for any fixed value of \mathcal{N}) the set (A19) and (A20) describes an exact QHD system evaluated in correspondence with a complete Moyal expansion of the kinetic Wigner equation.

By considering the left-hand side of equation system (A19) and (A20) we obtain the traceless moments

$$M_{(s)|(ik)} = M_{(s)ik} - \frac{2}{3} \frac{1}{m} M_{(s+1)} \delta_{ik},$$

$$M_{(s-1)|(ijk)} = M_{(s-1)ijk} - \frac{6}{5} \frac{1}{m} M_{(s)|(i} \delta_{jk)}.$$

Analogously, for increasing values of \mathcal{N} , in the right-hand side of Eqs. (A19) and (A20) we have also some traceless moments of higher tensorial order $M_{(l)|(i_1 \dots i_r)}$ with $r \geq 4$. Thus, the previous set of equations contains unknown constitutive functions H_A that, through Eq. (26)₂, are represented by the central moments of higher order with respect to the scalar and vectorial macroscopic variables, where

$$H_A = \{M_{(\mathcal{N}+1)}, M_{(l)|(ij)}, M_{(q)|(ijk)}, M_{(s)|(i_1 \dots i_r)}\}. \quad (\text{A24})$$

4. Moyal expansion for the phase space function $F(\tau, \mathbf{r}, \mathbf{p}) = \mathcal{W}(e^{\tau \hat{A}})$

Let us consider the operator $\hat{A}(\hat{\mathbf{r}}, \hat{\mathbf{p}})$ and the corresponding phase-space function $A(\mathbf{r}, \mathbf{p})$. By introducing an arbitrary scalar parameter τ , we define a new operator $\hat{F}(\tau, \hat{\mathbf{r}}, \hat{\mathbf{p}}) = e^{\tau \hat{A}(\hat{\mathbf{r}}, \hat{\mathbf{p}})}$ and the associated phase-space function $F(\tau, \mathbf{r}, \mathbf{p}) = \mathcal{W}(e^{\tau \hat{A}})$. Then one can show that F satisfies the relation

$$\frac{dF}{d\tau} = \mathcal{W}(\hat{A} \hat{F}), \quad (\text{A25})$$

with the condition $[\hat{A}, \hat{F}] = 0$ and $F(\tau, \mathbf{r}, \mathbf{p})|_{\tau=0} = \mathcal{W}(\hat{I}) = 1$.

The determination of $F(\tau, \mathbf{r}, \mathbf{p})$, as solution of Eq. (A25), can be obtained within different levels of approximation [11]. In particular, by using the Moyal formalism one can prove [45,51,52] that the Wigner function can be expanded in an even power of \hbar . Furthermore, for a correct evaluation of the reduced Wigner function under equilibrium and nonequilibrium conditions in terms of Lagrange multipliers, it is necessary to assume [6] that $\lambda_A(\mathbf{r}, \mathbf{p})$ can also be expanded in a power of \hbar^2 . Thus, for a correct evaluation of the phase space function $F(\tau, \mathbf{r}, \mathbf{p})$ in powers of \hbar we must consider, as general solutions of Eq. (A25), the solutions in which the phase-space function $A(\mathbf{r}, \mathbf{p})$ is expanded in an even power of \hbar , where

$$A(\mathbf{r}, \mathbf{p}) = \sum_{r=0}^{\infty} \hbar^{2r} A_{2r}(\mathbf{r}, \mathbf{p}). \quad (\text{A26})$$

In this case, by searching the solutions of Eq. (A25) in the form $F(\tau, \mathbf{r}, \mathbf{p}) = \sum \hbar^r F_r(\tau, \mathbf{r}, \mathbf{p})$, by using Eqs. (A26) and (A5) we obtain

$$\frac{dF_r}{d\tau} = \sum_{s=0}^{[r/2]} \sum_{l=0}^{[(r-2s)/2]} A_{2s} \star_{2l} F_{r-2(s+l)} \quad \text{with} \quad F_r|_{\tau=0} = \delta_{r0} \quad \forall r \geq 0, \quad (\text{A27})$$

where the symbol $[r/2]$ indicates the greatest integer $\leq r/2$.

By induction, one can readily verify that all odd terms F_{2r+1} vanish. Indeed, by solving Eq. (A27) for $r = 1$, we obtain that $F_1(\tau, \mathbf{r}, \mathbf{p}) = 0$. Analogously, if we formulate the *inductive hypothesis* that $F_{2l+1}(\tau, \mathbf{r}, \mathbf{p}) = 0$ for all $0 \leq l \leq \bar{r}$, then, by solving Eq. (A27), it is easy to prove that $F_{2\bar{r}+3}(\tau, \mathbf{r}, \mathbf{p}) = 0$. As a consequence, it is $F_{2r+1}(\tau, \mathbf{r}, \mathbf{p}) = 0 \quad \forall r \geq 0$. Analogously, one can solve Eq. (A27) for the even terms F_{2r} , obtaining the expansion

$$F(\tau, \mathbf{r}, \mathbf{p}) = \sum_{r=0}^{\infty} \hbar^{2r} F_{2r}(\tau, \mathbf{r}, \mathbf{p}) \quad \text{with} \quad F_{2r} = C_{2r}(\tau, \mathbf{r}, \mathbf{p}) e^{\tau A_0(\mathbf{r}, \mathbf{p})}, \quad (\text{A28})$$

where, for $r = 0$ it is $C_0 = 1$, while for $r \geq 1$ the functions C_{2r} are solutions of the equation

$$C'_{2r}(\tau, \mathbf{r}, \mathbf{p}) = \sum_{m=0}^{r-1} \sum_{s=1}^{r-m} \{A_{2m} \star_{2s} F_{2(r-m-s)}(\tau, \mathbf{r}, \mathbf{p})\} e^{-\tau A_0} + \sum_{m=1}^r A_{2m} C_{2(r-m)}(\tau, \mathbf{r}, \mathbf{p}). \quad (\text{A29})$$

It is further possible to show that the quantities C_{2r} are polynomial functions in the τ parameter with coefficients $\mathcal{H}_\alpha^{(2r)}(\mathbf{r}, \mathbf{p})$, being

$$C_{2r}(\tau, \mathbf{r}, \mathbf{p}) = \sum_{\alpha=0}^{3r} \tau^\alpha \mathcal{H}_\alpha^{(2r)}(\mathbf{r}, \mathbf{p}) \quad \text{with} \quad \mathcal{H}_0^{(2r)} = \delta_{r,0}. \quad (\text{A30})$$

Thus, for $r \geq 1$, we obtain the general recurrence formula

$$C_{2r}(\tau, \mathbf{r}, \mathbf{p}) = \int_0^\tau d\xi g_{2r}(\xi, \mathbf{r}, \mathbf{p}) + \sum_{m=1}^r A_{2m} \int_0^\tau d\xi C_{2(r-m)}(\xi, \mathbf{r}, \mathbf{p}), \quad (\text{A31})$$

where

$$g_{2r}(\xi, \mathbf{r}, \mathbf{p}) = \sum_{m=0}^{r-1} \sum_{s=1}^{r-m} \{A_{2m} \star_{2s} F_{2(r-m-s)}(\xi, \mathbf{r}, \mathbf{p})\} e^{-\xi A_0}. \quad (\text{A32})$$

As an example, for $r = 1$ it is

$$\int_0^\tau d\xi g_2(\xi, \mathbf{r}, \mathbf{p}) = Q_2(\tau, \mathbf{r}, \mathbf{p}) = \mathcal{H}_3^{(2)}(\mathbf{r}, \mathbf{p})\tau^3 + \mathcal{H}_2^{(2)}(\mathbf{r}, \mathbf{p})\tau^2, \quad (\text{A33})$$

with

$$\mathcal{H}_3^{(2)} = -\frac{1}{24} \left[\frac{\partial^2 A_0}{\partial x_i \partial x_j} \frac{\partial A_0}{\partial p_i} \frac{\partial A_0}{\partial p_j} + \frac{\partial^2 A_0}{\partial p_i \partial p_j} \frac{\partial A_0}{\partial x_i} \frac{\partial A_0}{\partial x_j} - 2 \frac{\partial^2 A_0}{\partial x_i \partial p_j} \frac{\partial A_0}{\partial x_j} \frac{\partial A_0}{\partial p_i} \right], \quad (\text{A34})$$

$$\mathcal{H}_2^{(2)} = -\frac{1}{8} \left[\frac{\partial^2 A_0}{\partial x_i \partial x_j} \frac{\partial^2 A_0}{\partial p_i \partial p_j} - \frac{\partial^2 A_0}{\partial x_i \partial p_j} \frac{\partial^2 A_0}{\partial x_j \partial p_i} \right], \quad (\text{A35})$$

and

$$C_2 = Q_2(\tau, \mathbf{r}, \mathbf{p}) + A_2(\mathbf{r}, \mathbf{p})\tau. \quad (\text{A36})$$

Therefore, by using cyclically Eqs. (A31) and (A32), we obtain the Moyal expansion

$$F(\tau, \mathbf{r}, \mathbf{p}) = \mathcal{W}(e^{\tau \hat{A}}) = e^{\tau A_0(\mathbf{r}, \mathbf{p})} \sum_{r=0}^{+\infty} \hbar^{2r} C_{2r}(\tau, \mathbf{r}, \mathbf{p}). \quad (\text{A37})$$

One can show that the expansion (A37) can be rewritten in the convenient form

$$F(\tau, \mathbf{r}, \mathbf{p}) = \mathcal{W}(e^{\tau \hat{A}}) = e^{\tau A(\mathbf{r}, \mathbf{p})} \sum_{r=0}^{+\infty} \hbar^{2r} Q_{2r}(\tau, \mathbf{r}, \mathbf{p}), \quad (\text{A38})$$

where

$$Q_0 = 1 \quad \text{and} \quad Q_{2s}(\tau, \mathbf{r}, \mathbf{p}) = \sum_{q=1}^s \int_0^\tau d\xi g_{2q}(\xi, \mathbf{r}, \mathbf{p}) H_{2(s-q)}^-(\xi, \mathbf{r}, \mathbf{p}) \quad \forall s \geq 1, \quad (\text{A39})$$

with the quantities H_{2r}^- and g_{2r} expressed, respectively, by (A7) and (A32).

The relation (A38) can be proved by induction using two steps.

In a first step, the statement

$$C_{2r}(\tau, \mathbf{r}, \mathbf{p}) = \sum_{k=0}^r Q_{2k} H_{2(r-k)}^+ \quad (\text{A40})$$

is proven to be true for all $r \geq 0$, where H_{2r}^+ and Q_{2k} are given by (A7) and (A39). In particular, by using Eqs. (A7), (A36), and (A39), we verify that Eq. (A40) is true for $r = 0, 1$. Thus, if we formulate the *inductive hypothesis* that the quantities C_{2l} are expressed by Eq. (A40) for all $0 \leq l \leq \bar{r}$, then we prove the relation

$$C_{2(\bar{r}+1)}(\tau, \mathbf{r}, \mathbf{p}) = \sum_{k=0}^{\bar{r}+1} Q_{2k} H_{2(\bar{r}+1-k)}^+. \quad (\text{A41})$$

Indeed, by using Eq. (A31) and the inductive hypothesis, we obtain

$$\begin{aligned} C_{2(\bar{r}+1)}(\tau, \mathbf{r}, \mathbf{p}) &= \int_0^\tau d\xi g_{2(\bar{r}+1)}(\xi, \mathbf{r}, \mathbf{p}) + \sum_{m=1}^{\bar{r}+1} A_{2m} \int_0^\tau d\xi H_{2(\bar{r}+1-m)}^+(\xi, \mathbf{r}, \mathbf{p}) \\ &+ \sum_{m=1}^{\bar{r}} A_{2m} \sum_{k=1}^{\bar{r}+1-m} \int_0^\tau d\xi Q_{2k}(\xi, \mathbf{r}, \mathbf{p}) H_{2(\bar{r}+1-m-k)}^+(\xi, \mathbf{r}, \mathbf{p}). \end{aligned} \quad (\text{A42})$$

By introducing the functions V_{2s}^+ defined in Eq. (A10), it is

$$\begin{aligned} C_{2(\bar{r}+1)}(\tau, \mathbf{r}, \mathbf{p}) &= \int_0^\tau d\xi g_{2(\bar{r}+1)}(\xi, \mathbf{r}, \mathbf{p}) + \sum_{m=1}^{\bar{r}+1} A_{2m} V_{2(\bar{r}+1-m)}^+(\tau, \mathbf{r}, \mathbf{p}) \\ &+ \sum_{m=1}^{\bar{r}} A_{2m} \sum_{k=1}^{\bar{r}+1-m} \int_0^\tau d\xi Q_{2k}(\xi, \mathbf{r}, \mathbf{p}) [V_{2(\bar{r}+1-m-k)}^+(\xi, \mathbf{r}, \mathbf{p})]'. \end{aligned} \quad (\text{A43})$$

Thus, integrating by part the last term of Eq. (A43) and using Eq. (A39), we obtain

$$\begin{aligned} C_{2(\bar{r}+1)}(\tau, \mathbf{r}, \mathbf{p}) &= \int_0^\tau d\xi \left[g_{2(\bar{r}+1)} - \sum_{m=1}^{\bar{r}} A_{2m} \sum_{k=1}^{\bar{r}+1-m} V_{2(\bar{r}+1-m-k)}^+ \sum_{q=1}^k g_{2q} H_{2(k-q)}^- \right] \\ &+ \sum_{m=1}^{\bar{r}} A_{2m} \sum_{k=1}^{\bar{r}+1-m} Q_{2k}(\tau, \mathbf{r}, \mathbf{p}) V_{2(\bar{r}+1-m-k)}^+(\tau, \mathbf{r}, \mathbf{p}) + \sum_{m=1}^{\bar{r}+1} A_{2m} V_{2(\bar{r}+1-m)}^+(\tau, \mathbf{r}, \mathbf{p}). \end{aligned} \quad (\text{A44})$$

Finally, by using the algebraic recurrence relations (A11)–(A13) and (A39), it is

$$C_{2(\bar{r}+1)} = \sum_{k=1}^{\bar{r}+1} \int_0^\tau d\xi g_{2k}(\xi, \mathbf{r}, \mathbf{p}) H_{2(\bar{r}+1-k)}^-(\xi, \mathbf{r}, \mathbf{p}) + \sum_{k=0}^{\bar{r}} Q_{2k} H_{2(\bar{r}+1-k)}^+ = \sum_{k=0}^{\bar{r}+1} Q_{2k} H_{2(\bar{r}+1-k)}^+.$$

Therefore, since the relation (A41) is proven, then Eq. (A40) is true for all $r \geq 0$.

In a second step, by means of Eq. (A40) we rewrite the expansion (A37) as a Cauchy product of power series, and by using Eq. (A9)₁ we conclude that $F(\tau, \mathbf{r}, \mathbf{p})$ can be expressed in the form (A38).

a. Application to a Boltzmann gas

A straightforward application of previous results is the determination of the Wigner function in the case of a Boltzmann gas. Indeed, by using the kinetic fields (24), the constraints (26), and the set of Lagrange multipliers λ_A in the form (39), we can express $A(\mathbf{r}, \tilde{\mathbf{p}}, t)$ by means of the expansion

$$A(\mathbf{r}, \tilde{\mathbf{p}}, t) = \sum_{r=0}^{\infty} \hbar^{2r} A_{2r}(\mathbf{r}, \tilde{\mathbf{p}}, t), \quad \text{with} \quad A_{2r} = - \sum_{A=1}^N \lambda_A^{(2r)}(\mathbf{r}, t) \tilde{\mathcal{M}}_A(\tilde{\mathbf{p}}). \quad (\text{A45})$$

Accordingly, where $\mathcal{W}(\hat{\varrho}) = (2\pi\hbar)^3 \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}, t)$ and using the relations (35), (A37), and (A38) with $\tau = 1$, for a Boltzmann gas we determine the two equivalent expansions:

$$\mathcal{F}_{\mathcal{W}} = \tilde{y} \exp \left\{ - \sum_{A=1}^N \lambda_A^{(0)} \tilde{\mathcal{M}}_A \right\} \left\{ 1 + \sum_{r=1}^{\infty} \hbar^{2r} \tilde{C}_{2r} \right\}, \quad (\text{A46})$$

$$\mathcal{F}_{\mathcal{W}} = \tilde{y} \exp \left\{ - \sum_{A=1}^N \lambda_A \tilde{\mathcal{M}}_A \right\} \left\{ 1 + \sum_{r=1}^{\infty} \hbar^{2r} \tilde{Q}_{2r} \right\}, \quad (\text{A47})$$

where $\tilde{y} = y/(2\pi\hbar)^3$, $\tilde{C}_{2r} = C_{2r}(\tau, \mathbf{r}, \mathbf{p})|_{\tau=1}$, and $\tilde{Q}_{2r} = Q_{2r}(\tau, \mathbf{r}, \mathbf{p})|_{\tau=1}$ where $\{C_{2r}, Q_{2r}\}$ are expressed, respectively, through the general recurrence relations (A31), (A32), and (A39).

We notice that in next sections all the results that can be obtained in the framework of Boltzmann statistics are more conveniently determined as limit cases of the Fermi and Bose statistics.

5. Moyal expansion of the Wigner function for Fermi and Bose gases

By assuming $\tau = 1$, we consider all the results of the previous section for the operators $\widehat{A}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$, $\widehat{F}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}}) = e^{\widehat{A}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})}$ and for the associated space-phase function $A(\mathbf{r}, \mathbf{p})$, $F(\mathbf{r}, \mathbf{p})$. By defining the new operator

$$\widehat{Q}^\pm(\widehat{\mathbf{r}}, \widehat{\mathbf{p}}) = y [\widehat{F}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}}) \pm \widehat{I}]^{-1}, \quad (\text{A48})$$

where y is a suitable dimensionless constant describing spin degeneracy and $[\widehat{Q}^\pm, \widehat{F}] = 0$.

To calculate the Moyal expansion for the corresponding phase-space function $Q^\pm(\mathbf{r}, \mathbf{p})$, we consider the Weyl-Wigner transform of the product $\widehat{Q}^\pm (\widehat{F} \pm \widehat{I})$ by using Eq. (A5):

$$\mathcal{W}(\widehat{Q}^\pm (\widehat{F} \pm \widehat{I})) = \sum_{s=0}^{\infty} \hbar^{2s} Q^\pm(\mathbf{r}, \mathbf{p}) \star_{2s} (F(\mathbf{r}, \mathbf{p}) \pm 1) = y. \quad (\text{A49})$$

Here F is expressed as expansion in an even power of \hbar , and searching Q^\pm in the form

$$Q^\pm(\mathbf{r}, \mathbf{p}) = y \sum_{r=0}^{\infty} \hbar^r Q_r^\pm(\mathbf{r}, \mathbf{p}), \quad (\text{A50})$$

by Eq. (A49) we obtain all the terms of expansion (A50). In particular, by considering only terms associated with odd powers of \hbar , we find

$$Q_{2r+1}^\pm (F_0 \pm 1) + \sum_{m=0}^{r-1} \sum_{s=0}^{r-m} Q_{2m+1}^\pm \star_{2s} F_{2(r-m-s)} = 0 \quad \forall r \geq 0, \quad (\text{A51})$$

and, by induction, one can prove that for all the odd terms $Q_{2r+1}^\pm = 0 \quad \forall r \geq 0$. Indeed, for $r = 0$, by Eq. (A51) we obtain $Q_1^\pm = 0$. Thus, if we formulate the *inductive hypothesis* that $Q_{2l+1}^\pm = 0$ for all $0 \leq l \leq \bar{r}$, then, by using Eq. (A51), it follows that $Q_{2\bar{r}+3}^\pm = 0$. As a consequence, we find that all odd terms must satisfy the condition $Q_{2r+1}^\pm = 0 \quad \forall r \geq 0$.

Analogously, by considering the even powers of \hbar we find

$$Q_{2r}^\pm (F_0 \pm 1) + \sum_{m=0}^{r-1} Q_{2m}^\pm F_{2(r-m)} + \sum_{m=0}^{r-1} \sum_{s=1}^{r-m} Q_{2m}^\pm \star_{2s} F_{2(r-m-s)} = \delta_{r0} \quad \forall r \geq 0, \quad (\text{A52})$$

and the general solution of Eq. (A52) is given in the form

$$Q_{2r}^\pm = \frac{1}{e^{A_0(\mathbf{r}, \mathbf{p})} \pm 1} D_{2r}^\pm(\mathbf{r}, \mathbf{p}), \quad (\text{A53})$$

where, for $r = 0$, it is $D_0^\pm = 1$, while for $r \geq 1$ the functions D_{2r}^\pm are obtained by the general recurrence formula

$$D_{2r}^\pm(\mathbf{r}, \mathbf{p}) = - \left\{ \sum_{m=0}^{r-1} Q_{2m}^\pm F_{2(r-m)} + L_{2r}^\pm \right\} \quad \text{with} \quad L_{2r}^\pm = \sum_{m=0}^{r-1} \sum_{s=1}^{r-m} Q_{2m}^\pm \star_{2s} F_{2(r-m-s)}. \quad (\text{A54})$$

In particular, for $r = 1$ we obtain the first-order quantum correction

$$D_2^\pm(\mathbf{r}, \mathbf{p}) = P_2^\pm(\mathbf{r}, \mathbf{p}) - \left(\frac{e^{A_0(\mathbf{r}, \mathbf{p})}}{e^{A_0(\mathbf{r}, \mathbf{p})} \pm 1} \right) A_2(\mathbf{r}, \mathbf{p}), \quad (\text{A55})$$

where

$$P_2^\pm = - \left(\frac{e^{A_0}}{e^{A_0} \pm 1} \right) [\mathcal{H}_3^{(2)} + \mathcal{H}_2^{(2)}] + 2 \left(\frac{e^{A_0}}{e^{A_0} \pm 1} \right)^2 [3 \mathcal{H}_3^{(2)} + \mathcal{H}_2^{(2)}] - 6 \left(\frac{e^{A_0}}{e^{A_0} \pm 1} \right)^3 \mathcal{H}_3^{(2)}, \quad (\text{A56})$$

and the functions $\mathcal{H}_3^{(2)}$, $\mathcal{H}_2^{(2)}$ are expressed by relations (A34) and (A35).

Thus, by cyclically using the approach above, we determine the Moyal expansion

$$Q^\pm(\mathbf{r}, \mathbf{p}) = \mathcal{W}(\widehat{Q}^\pm) = \frac{y}{e^{A_0(\mathbf{r}, \mathbf{p})} \pm 1} \sum_{r=0}^{\infty} \hbar^{2r} D_{2r}^\pm(\mathbf{r}, \mathbf{p}). \quad (\text{A57})$$

One can prove that this expansion can be rewritten in the convenient form

$$\varrho^\pm(\mathbf{r}, \mathbf{p}) = \mathcal{W}(\widehat{\varrho}^\pm) = \frac{y}{e^{A(\mathbf{r}, \mathbf{p})} \pm 1} \sum_{r=0}^{\infty} \hbar^{2r} P_{2r}^\pm(\mathbf{r}, \mathbf{p}), \quad (\text{A58})$$

where

$$P_0^\pm = 1 \quad \text{and} \quad P_{2r}^\pm = - \left\{ e^{A_0(\mathbf{r}, \mathbf{p})} \left[\sum_{m=0}^{r-1} \varrho_{2m}^\pm \sum_{q=1}^{r-m} Q_{2q} H_{2(r-m-q)}^+ \right] + L_{2r}^\pm \right\} \quad \forall r \geq 1, \quad (\text{A59})$$

where the functions H_{2s}^+ and Q_{2s} are expressed by Eqs. (A7) and (A39) evaluated for $\tau = 1$.

Also in this case the equivalence of Eqs. (A57) and (A58) can be proved by induction in two steps.

In a first step we prove that the statement

$$D_{2r}^\pm(\mathbf{r}, \mathbf{p}) = \sum_{k=0}^r G_{2k}^\pm P_{2(r-k)}^\pm \quad (\text{A60})$$

is true for all $r \geq 0$, where the quantities G_{2r}^\pm are defined in Eq. (A8) with $\tau = 1$. Thus, we check that Eq. (A60) is true for $r = 0, 1$; we assume the *inductive hypothesis* that the functions D_{2l}^\pm are expressed by Eq. (A60) for all $0 \leq l \leq \bar{r}$, and we prove the relation

$$D_{2(\bar{r}+1)}^\pm(\mathbf{r}, \mathbf{p}) = \sum_{k=0}^{\bar{r}+1} G_{2k}^\pm P_{2(\bar{r}+1-k)}^\pm. \quad (\text{A61})$$

Indeed, by Eqs. (A28)₂ and (A40) we can write

$$F_{2(\bar{r}+1-m)} = e^{A_0(\mathbf{r}, \mathbf{p})} \left\{ \sum_{q=1}^{\bar{r}+1-m} Q_{2q} H_{2(\bar{r}+1-m-q)}^+ + H_{2(\bar{r}+1-m)}^+ \right\},$$

and by inserting this result in Eq. (A54)₁ and using Eq. (A59), we find

$$D_{2(\bar{r}+1)}^\pm = P_{2(\bar{r}+1)}^\pm - e^{A_0} \varrho_0^\pm H_{2(\bar{r}+1)}^+ - e^{A_0} \sum_{m=1}^{\bar{r}} \varrho_{2m}^\pm H_{2(\bar{r}+1-m)}^+, \quad (\text{A62})$$

where $\varrho_{2m}^\pm = \varrho_0^\pm D_{2m}^\pm$, and by using the inductive hypothesis we obtain

$$D_{2(\bar{r}+1)}^\pm = P_{2(\bar{r}+1)}^\pm - \varrho_0^\pm e^{A_0} \sum_{m=0}^{\bar{r}} G_{2m}^\pm H_{2(\bar{r}+1-m)}^+ - \varrho_0^\pm e^{A_0} \sum_{m=1}^{\bar{r}} H_{2(\bar{r}+1-m)}^+ \sum_{k=0}^{m-1} G_{2k}^\pm P_{2(m-k)}^\pm. \quad (\text{A63})$$

By considering for the last two terms the recurrence relations (A8) and (A14) (with $\tau = 1$) we determine Eq. (A61), and we conclude that the relation (A60) is true for all $r \geq 0$.

In a second step, by Eq. (A60) we rewrite the expansion (A57) as a Cauchy product of power series, and, using Eq. (A9)₂, we obtain the phase-space function $\varrho^\pm(\mathbf{r}, \mathbf{p})$ in the form (A58). Also in this case, if we consider the kinetic fields (24), the constraints (26), and the Lagrange multipliers (39), then we can define $A(\mathbf{r}, \tilde{\mathbf{p}}, t)$ in terms of the expansion

$$A(\mathbf{r}, \tilde{\mathbf{p}}, t) = \sum_{r=0}^{\infty} \hbar^{2r} A_{2r}(\mathbf{r}, \tilde{\mathbf{p}}, t), \quad \text{with} \quad A_{2r} = \sum_{A=1}^N \lambda_A^{(2r)}(\mathbf{r}, t) \tilde{\mathcal{M}}_A(\tilde{\mathbf{p}}). \quad (\text{A64})$$

Therefore, where $\mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}, t) = \mathcal{W}(\widehat{\varrho}^\pm)/(2\pi\hbar)^3$, by relations (34), (A57), and (A58) we determine the Wigner function for the Fermi and Bose gases by means of the two equivalent expansions:

$$\mathcal{F}_{\mathcal{W}} = \frac{\tilde{y}}{e^{\Pi_0} \pm 1} \left\{ 1 + \sum_{r=1}^{\infty} \hbar^{2r} D_{2r}^\pm \right\}, \quad \text{with} \quad \Pi_0 = \sum_{A=1}^N \lambda_A^{(0)} \tilde{\mathcal{M}}_A, \quad (\text{A65})$$

$$\mathcal{F}_{\mathcal{W}} = \frac{\tilde{y}}{e^{\Pi} \pm 1} \left\{ 1 + \sum_{r=1}^{\infty} \hbar^{2r} P_{2r}^\pm \right\}, \quad \text{with} \quad \Pi = \sum_{A=1}^N \lambda_A \tilde{\mathcal{M}}_A, \quad (\text{A66})$$

where $\tilde{y} = y/(2\pi\hbar)^3$ and $\{D_{2r}^\pm, P_{2r}^\pm\}$ are expressed by recursive formulas (A54) and (A59).

6. Explicit first-order quantum correction for the Fermi and Bose gases

By considering the first term of Eq. (A66) we evaluate the *zero-order iteration* and obtain the relations (41). In this case, (i) the moments M_A must satisfy the classic system, and (ii) the zero-order approximation for the Lagrange multipliers λ_A can be determined by considering the expansion (50) and inverting the relations (41)₂.

With this approach, for the Fermi and Bose gases we obtain the classic relations [1,7] (42). Analogously, by considering the successive term of the expansion (A66) we obtain

$$\mathcal{F}_{\mathcal{W}} = \frac{\tilde{y}}{e^{\pi} \pm 1} \{1 + \hbar^2 P_2^{\pm}\} \quad \text{with} \quad M_A + O(\hbar^4) = \int d^3 p \tilde{\mathcal{M}}_A \mathcal{F}_{\mathcal{W}}. \quad (\text{A67})$$

In this case, (i) the moments M_A are calculated up to the first-order quantum correction. (ii) The correction term P_2^{\pm} is evaluated, using the previous iteration, by means of Eqs. (A34), (A35), and (A56). (iii) The first-order approximation for the Lagrange multipliers is determined by considering the expansion (50) and by inverting the quantum relations (A67)₂. For this purpose, it is necessary to introduce the Fermi and the Bose integral functions

$$I_n^{\pm}(\alpha) = \int_0^{+\infty} \frac{x^n}{\exp(\alpha + x^2) \pm 1} dx \quad (\text{A68})$$

satisfying the differentiation property with the recurrence relation

$$\frac{d^r I_n^{\pm}(\alpha)}{d\alpha^r} = (-1)^r \frac{\Gamma(\frac{n+1}{2})}{\Gamma(\frac{n+1}{2} - r)} I_{n-2r}^{\pm}(\alpha), \quad (\text{A69})$$

where, in general, the functions $I_n^{\pm}(\alpha)$ can be analytically continued also for complex values [62] of n , and the relation (A69) cannot be necessarily restricted to positive values [62] of n . Thus, all functions $I_n^{\pm}(\alpha)$ with negative values of n are defined by means of (A69). In this case, by assuming that the nonlocal effects are due essentially to the spatial derivatives of the equilibrium Lagrange multipliers α and β , we determine both $\mathcal{F}_{\mathcal{W}|E}$ and the linearized nonequilibrium Wigner function $\mathcal{F}_{\mathcal{W}|NE}$ in the form (51)–(54). In particular, by defining $z = n/T^{3/2}$, all nonlocal coefficients $\{Q^{(k,l)}, Q_{(ij)}^{(k,l)}\}$ contained in Eqs. (51)–(54) are expressed by means of relations

$$Q^{(1,1)} = -2 \left(\frac{I_2^{\pm}}{I_0^{\pm}} \right)^2 \left(\frac{\partial \ln z}{\partial x_k} \right)^2 + O(\hbar^2), \quad (\text{A70})$$

$$Q^{(1,2)} = \frac{1}{3} \frac{I_2^{\pm}}{I_0^{\pm}} \left\{ \left[1 + \frac{I_2^{\pm}}{I_0^{\pm}} \frac{I_{-2}^{\pm}}{I_0^{\pm}} \right] \left(\frac{\partial \ln z}{\partial x_k} \right)^2 - \frac{\partial \ln z}{\partial x_k} \frac{\partial \ln T}{\partial x_k} + \frac{\partial^2 \ln z}{\partial x_k \partial x_k} \right\} + O(\hbar^2), \quad (\text{A71})$$

$$Q^{(1,3)} = -\frac{1}{24} \left\{ \left(\frac{\partial \ln T}{\partial x_k} \right)^2 - 2 \frac{\partial^2 \ln T}{\partial x_k \partial x_k} \right\} + O(\hbar^2), \quad (\text{A72})$$

$$Q^{(2,1)} = 3 \frac{I_2^{\pm}}{I_0^{\pm}} \left\{ \left[1 + \frac{I_2^{\pm}}{I_0^{\pm}} \frac{I_{-2}^{\pm}}{I_0^{\pm}} \right] \left(\frac{\partial \ln z}{\partial x_k} \right)^2 + \frac{\partial^2 \ln z}{\partial x_k \partial x_k} \right\} + O(\hbar^2), \quad (\text{A73})$$

$$Q^{(2,2)} = \frac{1}{4} \left\{ 3 \frac{\partial^2 \ln T}{\partial x_k \partial x_k} - \left(\frac{\partial \ln T}{\partial x_k} \right)^2 \right\} + O(\hbar^2), \quad (\text{A74})$$

$$Q_{(ij)}^{(1,4)} = \frac{I_2^{\pm}}{I_0^{\pm}} \left\{ \left[1 + \frac{I_2^{\pm}}{I_0^{\pm}} \frac{I_{-2}^{\pm}}{I_0^{\pm}} \right] \frac{\partial \ln z}{\partial x_{(i}} \frac{\partial \ln z}{\partial x_{j)}} + \frac{\partial^2 \ln z}{\partial x_{(i} \partial x_{j)}} + 2 \frac{\partial \ln z}{\partial x_{(i}} \frac{\partial \ln T}{\partial x_{j)}} \right\} + O(\hbar^2), \quad (\text{A75})$$

$$Q_{(ij)}^{(1,5)} = \frac{1}{4} \left\{ \frac{\partial^2 \ln T}{\partial x_{(i} \partial x_{j)}} + \frac{\partial \ln T}{\partial x_{(i}} \frac{\partial \ln T}{\partial x_{j)}} \right\} + O(\hbar^2), \quad (\text{A76})$$

$$Q_{(ij)}^{(2,4)} = \frac{3}{2} \frac{\partial \ln T}{\partial x_{(i}} \frac{\partial \ln T}{\partial x_{j)}} + O(\hbar^2). \quad (\text{A77})$$

Finally, when all terms associated to the spatial derivatives of temperature are negligible respect to terms connected with the spatial derivatives of numerical density [53], then we have the *density-gradient approximation*. In this case we obtain that $Q^{(1,3)} = Q^{(2,2)} = Q_{(ij)}^{(1,5)} = Q_{(ij)}^{(2,4)} \approx 0$, while, for the remaining quantities, we find the quantities

$$Q^{(1)} = Q^{(1,1)}, \quad Q^{(2)} = Q^{(1,2)} = \frac{1}{9} Q^{(2,1)}, \quad Q_{(ij)} = Q_{(ij)}^{(1,4)}, \quad (\text{A78})$$

as explicitly reported in Appendix A of Ref. [6].

a. Nonequilibrium Lagrange multipliers and the closure problem for Fermi and Bose gases

To determine the nonequilibrium Lagrange multipliers and the constitutive relations, we define the matrices $\Upsilon_{ls}^{(r)}, \Upsilon_{ls}^{(r,i,j)} = \{\Upsilon_{ls}^{(r,1,1)}, \Upsilon_{ls}^{(r,1,2)}, \Upsilon_{ls}^{(r,1,3)}, \Upsilon_{ls}^{(r,2,1)}, \Upsilon_{ls}^{(r,2,2)}\}$ with $r = 0, 1$ and, $\Upsilon_{ls}^{(p,q)} = \{\Upsilon_{ls}^{(1,4)}, \Upsilon_{ls}^{(2,4)}, \Upsilon_{ls}^{(1,5)}\}$, $\tilde{\Upsilon}_{ls}^{(p,q)} = \{\tilde{\Upsilon}_{ls}^{(1,4)}, \tilde{\Upsilon}_{ls}^{(2,4)}, \tilde{\Upsilon}_{ls}^{(1,5)}\}$, by means of relations

$$\Upsilon_{sl}^{(r)} = \frac{\Gamma(s+l+r+\frac{3}{2})}{\Gamma(s+l+r+\frac{1}{2})} \frac{I_{2(s+l+r)}^{\pm}}{I_2^{\pm}}, \quad (\text{A79})$$

$$\Upsilon_{sl}^{(r,i,j)} = 2^{j-1} (-1)^i \left\{ \frac{\Gamma(s+l+j+r+\frac{1}{2})}{\Gamma(s+l+i+j+r-\frac{9}{2})} \frac{I_{2(s+l+i+j+r-5)}^{\pm}}{I_2^{\pm}} - \frac{\Gamma(j+\frac{1}{2})}{\Gamma(i+j-\frac{7}{2})} \frac{\Gamma(s+l+r+\frac{3}{2})}{\Gamma(s+l+r+\frac{1}{2})} \frac{I_{2(s+l+r)}^{\pm}}{I_2^{\pm}} \frac{I_{2(i+j-4)}^{\pm}}{I_2^{\pm}} \right\}, \quad (\text{A80})$$

$$\Upsilon_{sl}^{(p,q)} = \frac{2^{q-2}}{5} (-1)^p \frac{\Gamma(s+l+q-\frac{1}{2})}{\Gamma(s+l+p+q-\frac{11}{2})} \frac{I_{2(s+l+p+q-6)}^{\pm}}{I_2^{\pm}}, \quad (\text{A81})$$

$$\tilde{\Upsilon}_{sl}^{(p,q)} = \frac{2^{q-2}}{5} (-1)^p \frac{\Gamma(s+l+q+\frac{1}{2})}{\Gamma(s+l+p+q-\frac{9}{2})} \frac{I_{2(s+l+p+q-5)}^{\pm}}{I_2^{\pm}}. \quad (\text{A82})$$

Thus, by introducing the nonequilibrium Wigner expansion (52) in the moments (87), we obtain the following linear system in the nonequilibrium variables $\{\Lambda_{(l)}, \Lambda_{(l)k}\}$:

$$\Delta_{(s)} + O(\hbar^4) = -n \sum_{l=0}^{\mathcal{N}} \left\{ \Upsilon_{sl}^{(0)} + \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[\sum_{j=1}^3 \Upsilon_{sl}^{(0,1,j)} \mathcal{Q}^{(1,j)} + \sum_{j=1}^2 \Upsilon_{sl}^{(0,2,j)} \mathcal{Q}^{(2,j)} \right] \right\} (k_B T)^{s+l} \Lambda_{(l)}, \quad (\text{A83})$$

$$M_{(s)li} + O(\hbar^4) = -\frac{2}{3} \frac{n}{m} \sum_{l=0}^{\mathcal{N}} \left\{ \Upsilon_{sl}^{(1)} \delta_{ik} + \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[\left(\sum_{j=1}^3 \Upsilon_{sl}^{(1,1,j)} \mathcal{Q}^{(1,j)} + \sum_{j=1}^2 \Upsilon_{sl}^{(1,2,j)} \mathcal{Q}^{(2,j)} \right) \delta_{ik} + \sum_{p=1}^2 \Upsilon_{sl}^{(p,4)} \mathcal{Q}_{(ik)}^{(p,4)} + \Upsilon_{sl}^{(1,5)} \mathcal{Q}_{(ik)}^{(1,5)} \right] \right\} (k_B T)^{s+l+1} \Lambda_{(l)k}, \quad (\text{A84})$$

This system can be inverted, and we obtain

$$\Lambda_{(l)} = -\frac{1}{n} \sum_{s=2}^{\mathcal{N}} \left\{ \Omega_{ls}^{(0)} - \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[\sum_{p=1}^3 \Omega_{ls}^{(0,1,p)} \mathcal{Q}^{(1,p)} + \sum_{q=1}^2 \Omega_{ls}^{(0,2,q)} \mathcal{Q}^{(2,q)} \right] \right\} \left(\frac{1}{k_B T} \right)^{l+s} \Delta_{(s)} + O(\hbar^4), \quad (\text{A85})$$

$$\Lambda_{(l)k} = -\frac{3}{2} \frac{m}{n} \sum_{s=1}^{\mathcal{N}} \left\{ \Omega_{ls}^{(1)} \delta_{ki} - \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[\left(\sum_{p=1}^3 \Omega_{ls}^{(1,1,p)} \mathcal{Q}^{(1,p)} + \sum_{q=1}^2 \Omega_{ls}^{(1,2,q)} \mathcal{Q}^{(2,q)} \right) \delta_{ki} + \sum_{q=1}^2 \Omega_{ls}^{(q,4)} \mathcal{Q}_{(ki)}^{(q,4)} + \Omega_{ls}^{(1,5)} \mathcal{Q}_{(ki)}^{(1,5)} \right] \right\} \left(\frac{1}{k_B T} \right)^{l+s+1} M_{(s)li} + O(\hbar^4), \quad (\text{A86})$$

where all matrices $\Omega_{ls}^{(r)}, \Omega_{ls}^{(r,i,j)} = \{\Omega_{ls}^{(r,1,1)}, \Omega_{ls}^{(r,1,2)}, \Omega_{ls}^{(r,1,3)}, \Omega_{ls}^{(r,2,1)}, \Omega_{ls}^{(r,2,2)}\}$ obtained for $r = 0, 1$, and $\Omega_{ls}^{(p,q)} = \{\Omega_{ls}^{(1,4)}, \Omega_{ls}^{(2,4)}, \Omega_{ls}^{(1,5)}\}$, contained in these relations, are expressed in the form

$$\Omega_{ls}^{(r)} = (\Upsilon_{ls}^{(r)})^{-1}, \quad \Omega_{ls}^{(r,i,j)} = \Omega_{ln}^{(r)} \Upsilon_{nm}^{(r,i,j)} \Omega_{ms}^{(r)}, \quad \Omega_{ls}^{(p,q)} = \Omega_{ln}^{(1)} \Upsilon_{nm}^{(p,q)} \Omega_{ms}^{(1)}. \quad (\text{A87})$$

From the knowledge of the Lagrange multipliers, and using the matrices (A79)–(A82) and (A87), the constitutive relations are obtained through Eqs. (88)–(90), where all the coefficients $\zeta_{(\mathcal{N}+1)s} = \{\zeta_{(\mathcal{N}+1)s}^{(1,1)}, \zeta_{(\mathcal{N}+1)s}^{(1,2)}, \zeta_{(\mathcal{N}+1)s}^{(1,3)}, \zeta_{(\mathcal{N}+1)s}^{(2,1)}, \zeta_{(\mathcal{N}+1)s}^{(2,2)}\}$, $\xi_{sr}^{(p,q)} = \{\xi_{sr}^{(1,4)}, \xi_{sr}^{(2,4)}, \xi_{sr}^{(1,5)}\}$, and $\Phi_{sr}^{(p,q)} = \{\Phi_{sr}^{(1,4)}, \Phi_{sr}^{(2,4)}, \Phi_{sr}^{(1,5)}\}$, entering these relations, are given by

$$\zeta_{(\mathcal{N}+1)s} = \sum_{l=0}^{\mathcal{N}} \Upsilon_{(\mathcal{N}+1)l}^{(0)} \Omega_{ls}^{(0)}, \quad \zeta_{(\mathcal{N}+1)s}^{(i,j)} = \sum_{l=0}^{\mathcal{N}} [\Upsilon_{(\mathcal{N}+1)l}^{(0,i,j)} \Omega_{ls}^{(0)} - \Upsilon_{(\mathcal{N}+1)l}^{(0)} \Omega_{ls}^{(0,i,j)}], \quad (\text{A88})$$

$$\xi_{sr}^{(p,q)} = (k_B T)^{s-r} \sum_{l=0}^{\mathcal{N}} \Upsilon_{sl}^{(p,q)} \Omega_{lr}^{(0)}, \quad \Phi_{sr}^{(p,q)} = (k_B T)^{s-r} \sum_{l=0}^{\mathcal{N}} \tilde{\Upsilon}_{sl}^{(p,q)} \Omega_{lr}^{(1)}. \quad (\text{A89})$$

7. Explicit first-order quantum correction for a Boltzmann gas

We recall that for $\alpha \gg 1$ the Fermi and/or Bose integral functions are expressed by means of relation $I_n^\pm(\alpha) \approx (1/2)\Gamma[(n+1)/2]\exp(-\alpha)$. Thus, by considering Eqs. (53) and (A70)–(A77), we obtain

$$L_{(n)}^\pm = (-1)^n e^{-\alpha - \beta \bar{\epsilon}}, \quad (\text{A90})$$

$$\mathcal{Q}^{(1)} = \mathcal{Q}^{(2,1)} - \mathcal{Q}^{(1,1)}, \quad \mathcal{Q}^{(2)} = \mathcal{Q}^{(2,2)} - \mathcal{Q}^{(1,2)}, \quad (\text{A91})$$

$$\mathcal{Q}^{(3)} = -\mathcal{Q}^{(1,3)}, \quad \mathcal{Q}_{(ij)}^{(4)} = \mathcal{Q}_{(ij)}^{(2,4)} - \mathcal{Q}_{(ij)}^{(1,4)}, \quad \mathcal{Q}_{(ij)}^{(5)} = -\mathcal{Q}_{(ij)}^{(1,5)}, \quad (\text{A92})$$

where all coefficients $\{\mathcal{Q}^{(r)}, \mathcal{Q}_{(ij)}^{(p)}\}$ can be evaluated explicitly by using the Boltzmann approximation for the functions $I_n^\pm(\alpha)$ in the relations (A91) and (A92).

As a consequence, the Moyal expansions (56)–(58) for a Boltzmann gas are obtained as a particular case of the Moyal expansions (51)–(54) for the Fermi and Bose gases under nondegenerate conditions.

a. Nonequilibrium Lagrange multipliers and the closure problem for a Boltzmann gas

In the framework of Boltzmann statistic, to determine the nonequilibrium Lagrange multipliers and, as a consequence, the constitutive relations, we define the following matrices $\{A_{sl}^{(r)}, A_{sl}^{(r,j)}, \mathcal{A}_{sl}^{(p)}, \tilde{\mathcal{A}}_{sl}^{(p)}\}$ and $\{B_{ls}^{(r)}, B_{ls}^{(r,j)}, \mathcal{B}_{ls}^{(p)}\}$, with $r = 0, 1, j = 2, 3$, and $p = 4, 5$:

$$A_{sl}^{(r)} = \frac{[2(s+l+r)+1]!!}{2^{s+l+r}}, \quad A_{sl}^{(r,2)} = \frac{[2(s+l+r)+1]!!}{2^{s+l+r-1}}(s+l+r), \quad (\text{A93})$$

$$A_{sl}^{(r,3)} = \frac{[2(s+l+r)+1]!!}{2^{s+l+r-2}}(s+l+r)(s+l+r+4), \quad (\text{A94})$$

$$\mathcal{A}_{sl}^{(p)} = \frac{1}{5} \frac{[2(s+l+p)-3]!!}{2^{s+l}}, \quad \tilde{\mathcal{A}}_{sl}^{(p)} = \frac{1}{5} \frac{[2(s+l+p)-1]!!}{2^{s+l+1}}, \quad (\text{A95})$$

$$B_{ls}^{(r)} = (A_{ls}^{(r)})^{-1}, \quad B_{ls}^{(r,j)} = B_{ln}^{(r)} A_{nm}^{(r,j)} B_{ms}^{(r)}, \quad \mathcal{B}_{ls}^{(p)} = B_{ln}^{(1)} \mathcal{A}_{nm}^{(p)} B_{ms}^{(1)}. \quad (\text{A96})$$

Therefore, by evaluating the relations (A79)–(A82) for $\alpha \gg 1$, one can verify that

$$\begin{aligned} \Upsilon_{sl}^{(r)} &= A_{sl}^{(r)}; \quad \Upsilon_{sl}^{(r,1,2)} = -\Upsilon_{sl}^{(r,2,2)} = -A_{sl}^{(r,2)}, \quad \Upsilon_{sl}^{(r,1,3)} = -A_{sl}^{(r,3)}, \quad \Upsilon_{sl}^{(r,1,1)} = \Upsilon_{sl}^{(r,2,1)} = 0; \\ \Upsilon_{sl}^{(1,4)} &= -\Upsilon_{sl}^{(2,4)} = -\mathcal{A}_{sl}^{(4)}, \quad \Upsilon_{sl}^{(1,5)} = -\mathcal{A}_{sl}^{(5)}, \quad \tilde{\Upsilon}_{sl}^{(1,4)} = -\tilde{\Upsilon}_{sl}^{(2,4)} = -\tilde{\mathcal{A}}_{sl}^{(4)}, \quad \tilde{\Upsilon}_{sl}^{(1,5)} = -\tilde{\mathcal{A}}_{sl}^{(5)}; \\ \Omega_{sl}^{(r)} &= B_{sl}^{(r)}; \quad \Omega_{sl}^{(r,1,2)} = -\Omega_{sl}^{(r,2,2)} = -B_{sl}^{(r,2)}, \quad \Omega_{sl}^{(r,1,3)} = -B_{sl}^{(r,3)}, \quad \Omega_{sl}^{(r,1,1)} = \Omega_{sl}^{(r,2,1)} = 0; \\ \Omega_{sl}^{(1,4)} &= -\Omega_{sl}^{(2,4)} = -\mathcal{B}_{sl}^{(4)}, \quad \Omega_{sl}^{(1,5)} = -\mathcal{B}_{sl}^{(5)}. \end{aligned}$$

As a consequence, by using Eqs. (A83), (A84), (A91), and (A92) we obtain the following linear system:

$$\Delta_{(s)} + O(\hbar^4) = -n \sum_{l=0}^{\mathcal{N}} \left\{ A_{sl}^{(0)} + \frac{\hbar^2}{12m} \frac{1}{k_B T} \sum_{j=2}^3 [A_{sl}^{(0,j)} \mathcal{Q}^{(j)}] \right\} (k_B T)^{s+l} \Lambda_{(l)}, \quad (\text{A97})$$

$$\begin{aligned} M_{(s)|i} + O(\hbar^4) &= -\frac{2}{3} \frac{n}{m} \sum_{l=0}^{\mathcal{N}} \left\{ A_{sl}^{(1)} \delta_{ik} + \frac{\hbar^2}{12m} \frac{1}{k_B T} [(A_{sl}^{(1,2)} \mathcal{Q}^{(2)} + A_{sl}^{(1,3)} \mathcal{Q}^{(3)}) \delta_{ik} \right. \\ &\quad \left. + \mathcal{A}_{sl}^{(4)} \mathcal{Q}_{(ik)}^{(4)} + \mathcal{A}_{sl}^{(5)} \mathcal{Q}_{(ik)}^{(5)}] \right\} (k_B T)^{s+l+1} \Lambda_{(l)|k}, \quad (\text{A98}) \end{aligned}$$

and, as solution of these relations, the Lagrange multipliers

$$\Lambda_{(l)} = -\frac{1}{n} \sum_{s=2}^{\mathcal{N}} \left\{ B_{ls}^{(0)} - \frac{\hbar^2}{12m} \frac{1}{k_B T} \sum_{j=2}^3 [B_{ls}^{(0,j)} \mathcal{Q}^{(j)}] \right\} \left(\frac{1}{k_B T} \right)^{l+s} \Delta_{(s)} + O(\hbar^4), \quad (\text{A99})$$

$$\begin{aligned} \Lambda_{(l)|k} &= -\frac{3}{2} \frac{m}{n} \sum_{s=1}^{\mathcal{N}} \left\{ B_{ls}^{(1)} \delta_{ki} - \frac{\hbar^2}{12m} \frac{1}{k_B T} [(B_{ls}^{(1,2)} \mathcal{Q}^{(2)} + B_{ls}^{(1,3)} \mathcal{Q}^{(3)}) \delta_{ki} \right. \\ &\quad \left. + \mathcal{B}_{ls}^{(4)} \mathcal{Q}_{(ki)}^{(4)} + \mathcal{B}_{ls}^{(5)} \mathcal{Q}_{(ki)}^{(5)}] \right\} \left(\frac{1}{k_B T} \right)^{l+s+1} M_{(s)|i} + O(\hbar^4). \quad (\text{A100}) \end{aligned}$$

Analogously, by introducing the following matrices:

$$\chi_{(\mathcal{N}+1)s} = \sum_{l=0}^{\mathcal{N}} A_{(\mathcal{N}+1)l}^{(0)} B_{ls}^{(0)}, \quad \chi_{(\mathcal{N}+1)s}^{(j)} = \sum_{l=0}^{\mathcal{N}} [A_{(\mathcal{N}+1)l}^{(0,j)} B_{ls}^{(0)} - A_{(\mathcal{N}+1)l}^{(0)} B_{ls}^{(0,j)}], \quad (\text{A101})$$

$$\xi_{sr}^{(p)} = (k_B T)^{s-r} \sum_{l=0}^{\mathcal{N}} \mathcal{A}_{sl}^{(p)} B_{lr}^{(0)}, \quad \Phi_{sr}^{(p)} = (k_B T)^{s-r} \sum_{l=0}^{\mathcal{N}} \tilde{\mathcal{A}}_{sl}^{(p)} B_{lr}^{(1)}, \quad (\text{A102})$$

for $j = 2, 3$ and $p = 4, 5$, we consider Eqs. (A88) and (A89) to obtain the relations

$$\begin{aligned} \zeta_{(\mathcal{N}+1)s} &= \chi_{(\mathcal{N}+1)s}; & \zeta_{(\mathcal{N}+1)s}^{(1,2)} &= -\zeta_{(\mathcal{N}+1)s}^{(2,2)} = -\chi_{(\mathcal{N}+1)s}^{(2)}, & \zeta_{(\mathcal{N}+1)s}^{(1,3)} &= -\chi_{(\mathcal{N}+1)s}^{(3)}, \\ \zeta_{(\mathcal{N}+1)s}^{(1,1)} &= \zeta_{(\mathcal{N}+1)s}^{(2,1)} = 0; & \xi_{sl}^{(1,4)} &= -\xi_{sl}^{(2,4)} = -\xi_{sl}^{(4)}, & \xi_{sl}^{(1,5)} &= -\xi_{sl}^{(5)}, & \Phi_{sl}^{(1,4)} &= -\Phi_{sl}^{(2,4)} = -\Phi_{sl}^{(4)}, & \Phi_{sl}^{(1,5)} &= -\Phi_{sl}^{(5)}. \end{aligned}$$

As a consequence, all nonequilibrium closure relations (92)–(95) can be estimated under nondegenerate conditions by means of Eqs. (88)–(91).

-
- [1] I. Müller and T. Ruggeri, *Rational Extended Thermodynamics*, Springer Tracts in Natural Philosophy, Vol. 37 (Springer-Verlag, New York, 1998).
- [2] M. Trovato and P. Falsaperla, *Phys. Rev. B* **57**, 4456 (1998); M. Trovato and L. Reggiani, *ibid.* **61**, 16667 (2000); **73**, 245209 (2006), and references therein.
- [3] S. A. Gardiner, D. Jaksch, R. Dum, J. I. Cirac, and P. Zoller, *Phys. Rev. A* **62**, 023612 (2000).
- [4] K. H. Hughes, S. M. Parry, and I. Burghardt, *J. Chem. Phys.* **130**, 054115 (2009).
- [5] M. Trovato and L. Reggiani, *J. Phys. A* **43**, 102001 (2010).
- [6] M. Trovato and L. Reggiani, *Phys. Rev. E* **81**, 021119 (2010).
- [7] W. Dreyer, *J. Phys. A* **20**, 6505 (1987).
- [8] D. Jou, J. Casas-Vazquez, and G. Lebon, *Extended Irreversible Thermodynamics* (Springer-Verlag, New York, 2010).
- [9] E. T. Jaynes, *Phys. Rev.* **106**, 620 (1957); **108**, 171 (1957).
- [10] Y. Alhassid and R. D. Levine, *J. Chem. Phys.* **67**, 4321 (1977); *Phys. Rev. A* **18**, 89 (1978).
- [11] P. Degond and C. Ringhofer, *J. Stat. Phys.* **112**, 587 (2003); P. Degond, F. Mehats, and C. Ringhofer, *ibid.* **118**, 625 (2005).
- [12] C. Chamon, M. Oshikawa, and I. Affleck, *Phys. Rev. Lett.* **91**, 206403 (2003); A. Bulgac, *ibid.* **89**, 050402 (2002); G. Manfredi and P. A. Hervieux, *ibid.* **97**, 190404 (2006).
- [13] M. Kobayashi and M. Tsubota, *Phys. Rev. Lett.* **94**, 65302 (2005).
- [14] M. Müller, J. Schmalian, and L. Fritz, *Phys. Rev. Lett.* **103**, 025301 (2009); G. Bertaina, L. Pitaevskii, and S. Stringari, *ibid.* **105**, 150402 (2010); M. Olshanii, H. Perrin, and V. Lorent, *ibid.* **105**, 095302 (2010).
- [15] V. B. Eltsov, A. P. Finne, R. Hanninen, J. Kopu, M. Krusius, M. Tsubota, and E. V. Thuneberg, *Phys. Rev. Lett.* **96**, 215302 (2006); A. Bourne, N. K. Wilkin, and J. M. F. Gunn, *ibid.* **96**, 240401 (2006).
- [16] V. G. Kartavenko, *Yad. Fiz.* **40**, 377 (1984) [*Sov. J. Nucl. Phys.* **40**, 240 (1984)].
- [17] W. Frensky, *Rev. Mod. Phys.* **62**, 745 (1990).
- [18] A. Wettstein, A. Schenk, and W. Fichtner, *IEEE Trans. Electron. Devices* **48**, 279 (2001); D. Connelly, Z. Yu, and D. Yergeau, *ibid.* **49**, 619 (2002); M. G. Ancona and A. Svizhenko, *J. Appl. Phys.* **104**, 073726 (2008); M. G. Ancona, *J. Comput. Electron.* **10**, 65 (2011).
- [19] H. Tsuchiya, M. Horino, and T. Miyoshi, *J. Comput. Electron.* **2**, 91 (2003); A. Asenov, A. R. Brown, G. Roy, B. Cheng, C. Alexander, C. Riddet, U. Kovac, A. Martinez, N. Seoane, and S. Roy, *ibid.* **8**, 349 (2009); A. R. Brown, J. R. Watling, G. Roy, C. Riddet, C. L. Alexander, U. Kovac, A. Martinez, and A. Asenov, *ibid.* **9**, 187 (2010).
- [20] V. A. Cimmelli, A. Sellitto, and D. Jou, *Phys. Rev. B* **81**, 054301 (2010); **82**, 184302 (2010); D. Jou, G. Lebon, and M. Criado-Sancho, *Phys. Rev. E* **82**, 031128 (2010); G. Chen, *Nanoscale Energy Transport and Generation* (Oxford University Press, Oxford, 2005).
- [21] P. Kim, L. Shi, A. Majumdar, and P. L. McEuen, *Phys. Rev. Lett.* **87**, 215502 (2001); D. G. Cahill, W. K. Ford, K. E. Goodson, G. D. Mahan, A. Majumdar, H. J. Maris, R. Merlin, and S. R. Phillpot, *J. Appl. Phys.* **93**, 793 (2003); M. Fujii, X. Zhang, H. Xie, H. Ago, K. Takahashi, T. Ikuta, H. Abe, and T. Shimizu, *Phys. Rev. Lett.* **95**, 065502 (2005); Q. Z. Xue, *Nanotechnology* **17**, 1655 (2006).
- [22] Y. Cui and M. Lieber, *Science* **291**, 851 (2001); P. Yang, Y. Wu, and R. Fan, *Int. J. Nanosci.* **1**, 1 (2002); L. Willingale *et al.*, *Phys. Rev. Lett.* **105**, 095001 (2010).
- [23] M. G. Ancona and H. F. Tiersten, *Phys. Rev. B* **35**, 7959 (1987); M. G. Ancona and G. J. Iafrate, *ibid.* **39**, 9536 (1989).
- [24] C. Gardner, *SIAM J. Appl. Math.* **54**, 409 (1994); C. L. Gardner and C. Ringhofer, *Phys. Rev. E* **53**, 157 (1996).
- [25] A. S. Kompaneets and E. S. Pavlovskii, *Zh. Eksp. Teor. Fiz.* **31**, 427 (1956) [*Sov. Phys. JETP* **4**, 328 (1957)]; P. Hohenberg and W. Kohn, *Phys. Rev.* **136**, B864 (1964); F. Perrot, *Phys. Rev. A* **20**, 586 (1979).
- [26] C. C. Shih, *Phys. Rev. A* **14**, 919 (1976); N. L. Allan, C. G. West, D. L. Cooper, P. J. Grout, and N. H. March, *J. Chem. Phys.* **33**, 4562 (1985); E. Engel, P. LaRocca, and R. M. Dreizler, *Phys. Rev. B* **49**, 16728 (1994).
- [27] R. G. Parr and W. Yang, *Density-Functional Theory of Atoms and Molecules* (Oxford University Press, Oxford, 1994).
- [28] For the sake of simplicity, in the text we neglect the explicit dependence on time, being in general $\Psi(\mathbf{r}) = \Psi(\mathbf{r}, t)$ and $U(\mathbf{r}) = U(\mathbf{r}, t)$. Consequently, the quantities $\mathcal{H} = \mathcal{H}(\mathbf{r}, \mathbf{p}, t)$, $\langle \mathbf{r} | \hat{Q} | \mathbf{r}' \rangle = \langle \Psi(\mathbf{r}', t) | \Psi(\mathbf{r}, t) \rangle$, and $\mathcal{F}_{\mathcal{W}} = \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}, t)$ will also depend explicitly on t .

- [29] Yu. L. Klimontovich, Zh. Eksp. Teor. Fiz. **33**, 982 (1957) [Sov. Phys. JETP **6**, 753 (1958)]; W. E. Brittin and W. R. Chappell, *Rev. Mod. Phys.* **34**, 620 (1962); C. N. Yang, *ibid.* **34**, 694 (1962).
- [30] K. Imre, E. Ozizmir, M. Rosenbaum, and P. Zweifel, *J. Math. Phys.* **8**, 1097 (1967).
- [31] V. P. Silin, Zh. Eksp. Teor. Fiz. **33**, 495 (1957) [Sov. Phys. JETP **6**, 387 (1958)]; **35**, 1243 (1958) [**8**, 870 (1959)]; Yu. L. Klimontovich, *ibid.* **52**, 1233 (1967) [**25**, 820 (1967)]; Yu. L. Klimontovich and W. Ebeling, *ibid.* **63**, 905 (1972) [**36**, 476 (1973)].
- [32] H. Smith, H. H. Jensen, *Transport Phenomena* (Clarendon Press, Oxford, 1989).
- [33] A. S. Parkins and D. F. Walls, *Phys. Rep.* **303**, 1 (1998).
- [34] W. Ketterle and H. J. Miesner, *Phys. Rev. A* **56**, 3291 (1997); Yu. Kagan, B. V. Svistunov, and G. V. Shlyapnikov, Pis'ma Zh. Eksp. Teor. Fiz. **42**, 169 (1985) [JETP Lett. **42**, 209 (1985)].
- [35] M. Ploszajczak and M. J Rhoades-Brown, *Phys. Rev. Lett.* **55**, 147 (1985); *Phys. Rev. D* **33**, 3686 (1986).
- [36] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics*, Chap. 3, §3 (W. A. Benjamin, New York, 1962).
- [37] Yu. Klimontovich, *Kinetic Theory of Nonideal Gases and Nonideal Plasmas*, Part III, Vol. 105 (Pergamon Press, New York, 1982).
- [38] N. N. Bogouliov, J. Phys. (USSR) **10**, 265 (1946); N. N. Bogouliov and K. P. Gurov, Zh. Eksp. Teor. Fiz. **17**, 614 (1947).
- [39] F. Rossi and T. Kuhn, *Rev. Mod. Phys.* **74**, 895 (2002); H. W. Wyld and B. D. Fried, *Ann. Phys. (NY)* **23**, 374 (1963); D. B. Tran Thoai and H. Haug, *Phys. Rev. B* **47**, 3574 (1993); V. M. Axt and A. Stahl, *Z. Phys. B* **93**, 195 (1994).
- [40] M. Escobedo and J. J. L. Velázquez, *J. Phys. A* **41**, 395208 (2008).
- [41] Y. Castin and R. Dum, *Phys. Rev. A* **57**, 3008 (1998); E. Fersino, G. Mussardo, and A. Trombettoni, *ibid.* **77**, 053608 (2008).
- [42] J. V. Lill, M. I. Haftel, and G. H. Herling, *Phys. Rev. A* **39**, 5832 (1989); *J. Chem. Phys.* **90**, 4940 (1989); G. J. Iafrate, H. L. Grubin, and D. K. Ferry, *J. Physique C* **7** (Suppl. 10), 307 (1981).
- [43] J. Skilling, *Maximum Entropy and Bayesian Methods* (Kluwer Academic Publishers, Cambridge, 1988).
- [44] W. T. Grandy, *Principles of Statistical Mechanics*, Vols. 1 and 2 (Reidel, Dordrecht, 1987); H. Grabert, *Projection Operators Technique in Nonequilibrium Statistics* (Springer, New York, 1981); D. N. Zubarev, V. N. Morozov, and G. Röpke, *Statistical Mechanics of Nonequilibrium Processes*, Vols. 1 and 2 (Akademie Verlag, Berlin, 1996); R. Luzzi, A. R. Vasconcellos, and J. G. Ramos, *Predictive Statistical Mechanics: A Nonequilibrium Ensemble Formalism* (Kluwer, Dordrecht, 2002).
- [45] M. Hillery, R. O'Connell, M. Scully, and E. P. Wigner, *Phys. Rep.* **106**, 121 (1984).
- [46] J. Von Neumann, *The Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Princeton, 1955).
- [47] A. Wehrl, *Rev. Mod. Phys.* **50**, 221 (1978); E. P. Gyftopoulos and E. Çubukçu, *Phys. Rev. E* **55**, 3851 (1997); G. Manfredi and M. R. Feix, *ibid.* **62**, 4665 (2000).
- [48] A. Renyi, *Probability Theory* (North Holland, Amsterdam, 1970); C. Beck and F. Schlögl, *Thermodynamics of Chaotic Systems* (Cambridge University Press, Cambridge, 1993).
- [49] L. D. Landau and E. M. Lifshitz, *Statistical Physics*, Chap. V, §54, Vol. 5 (Pergamon Press, London, 1959).
- [50] J. E. Moyal, *Proc. Cambridge Phil. Soc.* **45**, 99 (1949).
- [51] E. P. Wigner, *Phys. Rev.* **40**, 749 (1932).
- [52] P. Carruthers and F. Zachariasen, *Rev. Mod. Phys.* **55**, 245 (1983).
- [53] Within this approximation, all terms containing the quantities $\frac{\partial \ln T}{\partial x_i}$ and $\frac{\partial^2 \ln T}{\partial x_i \partial x_j}$ in Eq. (54) can be neglected with respect to the remaining terms, and we obtain Eq. (55).
- [54] R. B. Lindsay, *Introduction to Physical Statistics* (John Wiley, Englewood Cliffs, NJ, 1958).
- [55] A. Sommerfeld, *Z. Physik* **47**, 1 (1928).
- [56] R. B. Dingle, *Asymptotic Expansions: Their Derivation and Interpretation* (Academic Press, New York, 1973).
- [57] For the electron gas in a strongly inhomogeneous condition, gradient corrections were introduced in the context of Thomas-Fermi-Weizsacker theory, using the density-functional approach [25–27]. Thus, by considering the usual density-gradient expansion of the total energy functional $\mathcal{T} = \int t[n(\mathbf{r}), \nabla n(\mathbf{r})] d\mathbf{r}$, we have $t = (t_{TF} + t_W/9)$, where $t_{TF} = (3/2)v_F n(\mathbf{r})^{5/3}$ is the Thomas-Fermi (TF) component and $t_W = (\hbar^2/8m)[\nabla n(\mathbf{r})]^2/n(\mathbf{r})$ is the original Weizsacker (W) correction. By minimizing the functional \mathcal{T} under the constraint of fixed number of fermions $\int n(\mathbf{r}) d\mathbf{r} = N$, we obtain the differential equation $\partial t/\partial n - \partial_k[\partial t/\partial(\partial_k n)] = \mu$, where the chemical potential μ is the Lagrange multiplier for the constraint. Within this approach we obtain $\mu = (5/2)v_F n(\mathbf{r})^{2/3} - \hbar^2/(72m)[2\Delta n(\mathbf{r})/n(\mathbf{r}) - (\nabla n(\mathbf{r}))^2/n(\mathbf{r})^2]$, which is exactly the expression (72)₁ for the chemical potential, where $Q_B = -\hbar^2/(8m)[2\Delta n(\mathbf{r})/n(\mathbf{r}) - (\nabla n(\mathbf{r}))^2/n(\mathbf{r})^2]$ is the quantum Bohm potential. Vice versa, by considering the relation (72)₂ it is easy to calculate, for the energy density, the expression $t_{CD} = t_{TF} + t_W/9 + (\hbar^2/24m)\Delta n(\mathbf{r})$. Since $\Delta n(\mathbf{r})$ integrates to zero (the Laplacian term is the divergence of a vector field that vanishes at infinity; thus, by Gauss's theorem, it does not contribute in the integral of total functional energy), we obtain the well-known density-gradient expansion for the total energy functional $\mathcal{T} = \int (t_{TF} + t_W/9) d\mathbf{r}$.
- [58] I. Gyarmati, E. Gyarmati, and W. F. Heinz, *Nonequilibrium Thermodynamics: Field Theory and Variational Principles* (Springer, New York, 1970); M. I. Shakhparonov, in *Nonequilibrium Process Thermodynamics* (in Russian) (Nauka, Moscow, 1987), p. 87.
- [59] R. P. Feynman and A. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw Hill, New York, 1965).
- [60] S. Reinecke and G. M. Kremer, *Phys. Rev. A* **42**, 815 (1990); *Continuum Mech. Thermodyn.* **3**, 155 (1991).
- [61] H. Struchtrup, *Continuum Mech. Thermodyn.* **9**, 23 (1997).
- [62] J. McDougall and E. C. Stoner, *Philos. Trans. R. Soc. London* **237**, 67 (1938); J. E. Robinson, *Phys. Rev.* **83**, 678 (1951).