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Quantum maximum entropy principle for a system of identical particles

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By introducing a functional of the reduced density matrix, we generalize the definition of a quantum entropy which incorporates the indistinguishability principle of a system of identical particles. With the present definition, the principle of quantum maximum entropy permits us to solve the closure problem for a quantum hydrodynamic set of balance equations corresponding to an arbitrary number of moments in the framework of extended thermodynamics. The determination of the reduced Wigner function for equilibrium and nonequilibrium conditions is found to become possible only by assuming that the Lagrange multipliers can be expanded in powers of $\hbar^2$. Quantum contributions are expressed in powers of $\hbar^2$ while classical results are recovered in the limit $\hbar \to 0$.

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I. INTRODUCTION

Entropy is a fundamental physical quantity to describe the properties of a statistical ensemble. Its microscopic definition was provided by Boltzmann through the celebrated expression $S = k_B \ln \Gamma$, where k_B is the Boltzmann constant and Γ is the number of microstates exploiting the same macroscopic properties. In the context of classical statistical mechanics, according to Gibbs, entropy can be expressed in terms of the phase-space probability distribution $f(\mathbf{r},\mathbf{p},t)$,

$$S_{cl} = -k_B \int d\sigma f \ln f, \tag{1}$$

with $d\sigma = d^3r d^3p/(2\pi\hbar)^3$. In this case, it is well known that (i) the classical entropy allows the violation of uncertainty principle [1,2], (ii) Eq. (1) can be considered as a special case of the so-called *Boltzmann-Gibbs-Shannon* entropy which enables one to apply results of information theory to physics [1,3]. In particular, by introducing the maximum entropy principle (MEP) it was found possible to derive rigorous hydrodynamic models based on the *moments* of the distribution function to all orders of the power expansion with their appropriate closure [4,5]. Accordingly, making use of the Lagrange multipliers technique, it was found possible to construct the set of evolution equations for the macrovariables of interest.

This is no longer the case under quantum nonlocal conditions, as pointed out in [6,7]. Here, the most used definition of entropy is the von Neumann expression

$$S = -k_B \operatorname{Tr}(\rho \ln \rho), \tag{2}$$

with ρ as the density matrix operator appropriate to the physical system under study. The definition above recovers the classical case when ρ is substituted by the classical distribution function. Although relation (2) does not refer to any special structure of a system, there are some particular features that must be satisfied for systems of identical particles. Indeed, a main drawback of the above definition, as well as of others [1,2,7], stems from the impossibility to account for the indistinguishability principle of a system of identical particles. To include the effects of indistinguishability in Eq. (2), it is mandatory to consider additional information specifying whether the density operator ρ, defined in the Fock space, is associated with a fermion or boson system.

The aim of this work is to address the above drawback by defining a quantum entropy in terms of the *reduced density matrix*, thus explicitly incorporating the statistics into problems involving a system of identical particles. As the second step, with respect to the uncertainty principle, starting from the Wigner representation we formulate a quantum maximum entropy principle (QMEP) which, in the framework of information theory, allows us to obtain a nonlocal theory for the system. As the third step, we determine a closed quantum hydrodynamic (QHD) system for the macroscopic variables used as constraints in the QMEP approach.

II. GENERAL THEORY AND RESULTS

We consider a fixed number N of identical particles introducing, in the Fock space [8], the general Hamiltonian

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

with many-body interactions, the statistical density matrix ρ, being $\operatorname{Tr}(\rho)=1$, and Ψ as the particle field operator satisfying the relations $[\Psi(\mathbf{r}),\Psi(\mathbf{r}')]_\pm = [\Psi^\dagger(\mathbf{r}),\Psi^\dagger(\mathbf{r}')]_\pm = 0$, $[\Psi(\mathbf{r}),\Psi^\dagger(\mathbf{r}')]_\pm = \delta(\mathbf{r}-\mathbf{r}')$ and the upper and lower signs refer to fermions and bosons.

Analogously, in the coordinate space representation we define the reduced density matrix [9] of single particle $\langle \mathbf{r}|\hat{\varrho}|\mathbf{r}'\rangle = \langle \Psi^\dagger(\mathbf{r}')\Psi(\mathbf{r})\rangle = \operatorname{Tr}[\rho\Psi^\dagger(\mathbf{r}')\Psi(\mathbf{r})]$ that in an arbitrary representation takes the form $\langle \nu|\hat{\varrho}|\nu'\rangle = \langle a^\dagger_{\nu'} a_\nu\rangle = \operatorname{Tr}(\rho a^\dagger_{\nu'} a_\nu)$ with ν, ν' being single-particle states; $a_\nu, a^\dagger_{\nu'}$ being the annihilation and creation operators for these states; and $\langle \cdots \rangle$ being the statistical mean value. From this formalism [9], we define the *reduced* Wigner function

$$\mathcal{F}_{\mathcal{W}} = \frac{1}{(2\pi\hbar)^3}\int d^3\tau e^{-(i/\hbar)\tau\cdot\mathbf{p}}\langle\Psi^\dagger(\mathbf{r}-\tau/2)\Psi(\mathbf{r}+\tau/2)\rangle, \quad (4)$$

obtaining for the momentum space distribution function $\int d^3r\mathcal{F}_{\mathcal{W}}=\langle\mathbf{p}|\hat{\varrho}|\mathbf{p}\rangle=\langle N_p\rangle$, and the dual expression $\int d^3p\mathcal{F}_{\mathcal{W}}=\langle\mathbf{r}|\hat{\varrho}|\mathbf{r}\rangle=n(\mathbf{r})$, where $\langle N_p\rangle$ is the mean occupation number and $n(\mathbf{r})$ is the quasiparticle numerical density, with $\mathrm{Tr}(\hat{\varrho})=N$. Accordingly, we look [10] for a function $\tilde{\mathcal{M}}(\mathbf{r},\mathbf{p})$ in phase space that *corresponds* unambiguously to an operator of single particle $\hat{\mathcal{M}}(\hat{\mathbf{r}},\hat{\mathbf{p}})$, introducing the Weyl-Wigner transform $\mathcal{W}(\hat{\mathcal{M}})=\tilde{\mathcal{M}}$. Analogously, we define the inverse Weyl-Wigner transform $\mathcal{W}^{-1}(\tilde{\mathcal{M}})=\langle\mathbf{r}|\hat{\mathcal{M}}|\mathbf{r}'\rangle$, being

$$\tilde{\mathcal{M}}(\mathbf{r},\mathbf{p}) = \int d^3\tau\langle\mathbf{r}+\tau/2|\hat{\mathcal{M}}|\mathbf{r}-\tau/2\rangle e^{-(i/\hbar)\tau\cdot\mathbf{p}},$$

$$\langle\mathbf{r}|\hat{\mathcal{M}}|\mathbf{r}'\rangle = \frac{1}{(2\pi\hbar)^3}\int d^3p\tilde{\mathcal{M}}\left(\frac{\mathbf{r}+\mathbf{r}'}{2},\mathbf{p}\right)e^{(i/\hbar)\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}.$$

Thus, $\tilde{\varrho}(\mathbf{r},\mathbf{p})=\mathcal{W}(\hat{\varrho})=(2\pi\hbar)^3\mathcal{F}_{\mathcal{W}}$, $\langle\mathbf{r}|\hat{\varrho}|\mathbf{r}'\rangle=\mathcal{W}^{-1}(\tilde{\varrho})$. To take into account *ab initio* the statistics for a system of identical particles, we follow the Landau strategy [11] and evaluate the entropy as the logarithm of the *statistical weight*. Thus, for a noninteracting system of fermions or bosons, in nonequilibrium conditions, the quantum entropy can be determined in terms of the occupation numbers by the form $S=-k_B\Sigma_\nu y[\overline{\langle N_\nu\rangle}\ln\overline{\langle N_\nu\rangle}\pm(1\mp\overline{\langle N_\nu\rangle})\ln(1\mp\overline{\langle N_\nu\rangle})]$, where $\overline{\langle N_\nu\rangle}=\langle a_\nu^\dagger a_\nu\rangle/y$, with $y=(2\tilde{s}+1)$ being the spin degeneration, and the upper and lower signs referring to fermions and bosons, respectively. If we consider the Schrodinger equation of single particle $[\hat{\mathcal{H}}(\mathbf{r})-E_\nu]\varphi_\nu(\mathbf{r})=0$, then the occupation numbers $\langle N_\nu\rangle$, associated with the energies E_ν, will completely specify the macroscopic state of the gas [11]. In particular, in stationary conditions, both the reduced density matrix and any operator $\hat{\Phi}(\hat{\varrho})$ are diagonal in the base φ_ν. Therefore, introducing as a function of $\hat{\varrho}$ the quantity

$$\hat{\Phi}(\hat{\varrho}) = \hat{\varrho}\left\{\ln\left(\frac{\hat{\varrho}}{y}\right) \pm y\hat{\varrho}^{-1}\left(\hat{I}\mp\frac{\hat{\varrho}}{y}\right)\ln\left(\hat{I}\mp\frac{\hat{\varrho}}{y}\right)\right\}, \quad (5)$$

with $\hat{I}$ as the identity, we obtain $\langle\nu|\hat{\varrho}|\nu'\rangle=\langle a_\nu^\dagger a_\nu\rangle\delta_{\nu\nu'}$ and $\langle\nu|\hat{\Phi}(\hat{\varrho})|\nu'\rangle=y[\overline{\langle N_\nu\rangle}\ln\overline{\langle N_\nu\rangle}\pm(1\mp\overline{\langle N_\nu\rangle})\ln(1\mp\overline{\langle N_\nu\rangle})]\delta_{\nu\nu'}$. Consequently, by generalizing existing definitions [1,2,7], the Bose or Fermi statistics can be implicitly taken into account by defining the quantum entropy for the whole system in terms of the functional of the reduced density operator

$$S(\hat{\varrho}) = -k_B\,\mathrm{Tr}[\hat{\Phi}(\hat{\varrho})], \quad (6)$$

with $\hat{\Phi}(\hat{\varrho})$ given by Eq. (5). By considering an arbitrary set of single-particle observable $\{\hat{\mathcal{M}}_A\}$ and the corresponding space-phase functions $\{\tilde{\mathcal{M}}_A\}$, the expectation values can be expressed by the *global* quantities

$$\langle\hat{\mathcal{M}}_A(\hat{\mathbf{r}},\hat{\mathbf{p}})\rangle = \int\int d^3pd^3r\tilde{\mathcal{M}}_A(\mathbf{r},\mathbf{p})\mathcal{F}_{\mathcal{W}}(\mathbf{r},\mathbf{p},t).$$

Analogously, we can define the macroscopic *local moments* $M_A(\mathbf{r},t)$ of $\hat{\mathcal{M}}_A(\hat{\mathbf{r}},\hat{\mathbf{p}})$ by means of the *local* relations

$$M_A(\mathbf{r},t) = \int d^3p\tilde{\mathcal{M}}_A(\mathbf{r},\mathbf{p})\mathcal{F}_{\mathcal{W}}(\mathbf{r},\mathbf{p},t),$$

and we use the functional (6) as an *informational entropy* for the system. To explicit the QMEP approach in phase space, we introduce the corresponding phase function $\tilde{\Phi}(\mathbf{r},\mathbf{p})=\mathcal{W}(\hat{\Phi})$, rewriting Eq. (6) as

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

and we search the extremal value of entropy subject to the constraint that the accessible information on the physical system is described by the set $\{M_A(\mathbf{r},t)\}$. To this purpose, we consider the global functional [7]

$$\tilde{S} = S - \int d^3r\left\{\sum_{A=1}^{N}\tilde{\lambda}_A\left[\int d^3p\tilde{\mathcal{M}}_A\mathcal{F}_{\mathcal{W}} - M_A\right]\right\}, \quad (7)$$

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

$$\hat{\varrho} = y\left\{\exp\left[\mathcal{W}^{-1}\left(\sum_{A=1}^{N}\lambda_A(\mathbf{r},t)\tilde{\mathcal{M}}_A\right)\right]\pm\hat{I}\right\}^{-1}, \quad (8)$$

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

Equation (8) is a first major result of the work since together with Eqs. (5) and (6) it provides a generalized definition of quantum entropy that includes particle indistinguishability. As a consequence, a nonlocal theory for the system can be formulated by explicitly evaluating the corresponding reduced Wigner function

$$\mathcal{F}_{\mathcal{W}} = \frac{1}{(2\pi\hbar)^3}\mathcal{W}(\hat{\varrho}[\lambda_A(\mathbf{r},t),\tilde{\mathcal{M}}_A]). \quad (9)$$

We remark that by using this approach in a dynamical context the information theory is not used as an extrapolation technique [12]. 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 between particles. Thus, using functional forms (8) and (9) of the reduced Wigner function, we determine the quantum kinetic equation for $\mathcal{F}_{\mathcal{W}}$ to obtain a set of equations for the constraints. This set completely represents the closed QHD model in which all the constitutive functions are determined starting from their kinetic expressions. Thus, knowing the correct dynamic evolution of the macroscopic quantities used as constraints it is possible to determine the correct dynamic evolution of the Wigner function in terms of Lagrange multipliers. Following a usual script [9,13], the equation of motion for the *reduced Wigner function* takes the compact form

$$i\hbar\frac{\partial}{\partial t}\mathcal{F}_{\mathcal{W}}(\mathbf{r},\mathbf{p}) = \int D\xi[\tilde{\mathcal{H}}(\mathbf{r}' + \tau/2,\mathbf{p}' + \phi/2) - \tilde{\mathcal{H}}(\mathbf{r}' - \tau/2,\mathbf{p}' - \phi/2)]\mathcal{F}_{\mathcal{W}}(\mathbf{r}',\mathbf{p}'), \tag{10}$$

where $D\xi = d^3r' d^3p' d^3\tau d^3\phi e^{(i/\hbar)[\tau\cdot(\mathbf{p}'-\mathbf{p})+\phi\cdot(\mathbf{r}-\mathbf{r}')]}$ and $\tilde{\mathcal{H}}$ is the phase function of single-particle operator $\hat{\mathcal{H}} = \langle\mathcal{H}\rangle$, being

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + \sum_{k=1}^{L-1}\frac{1}{k!}\int d^3r_1 \cdots \int d^3r_k \Psi^\dagger(\mathbf{r_1}) \times \cdots \Psi^\dagger(\mathbf{r_k})V(\mathbf{r},\mathbf{r_1},\ldots,\mathbf{r_k})\Psi(\mathbf{r_k})\cdots\Psi(\mathbf{r_1}). \tag{11}$$

Thus, the integrand function of Eq. (10) can be expressed as

$$\tilde{\mathcal{H}}\left(\mathbf{r}' + \frac{\tau}{2},\mathbf{p}' + \frac{\phi}{2}\right) - \tilde{\mathcal{H}}\left(\mathbf{r}' - \frac{\tau}{2},\mathbf{p}' - \frac{\phi}{2}\right) = \frac{p'_\alpha}{m}\phi_\alpha + V_{eff}\left(\mathbf{r}' + \frac{\tau}{2}\right) - V_{eff}\left(\mathbf{r}' - \frac{\tau}{2}\right), \tag{12}$$

where

$$V_{eff}(\mathbf{r}) = V(\mathbf{r}) + \sum_{k=1}^{L-1}\frac{1}{k!}\int d^3r_1 \cdots \int d^3r_k g^{(k)}(\mathbf{r_1},\ldots,\mathbf{r_k}) \times n(\mathbf{r_1})\cdots n(\mathbf{r_k})V(\mathbf{r},\mathbf{r_1},\ldots,\mathbf{r_k}), \tag{13}$$

with $g^{(k)}(\mathbf{r_1},\ldots,\mathbf{r_k})$ being the k-order correlation function

$$g^{(k)}(\mathbf{r_1},\ldots,\mathbf{r_k}) = \frac{\langle\Psi^\dagger(\mathbf{r_1})\cdots\Psi^\dagger(\mathbf{r_k})\Psi(\mathbf{r_k})\cdots\Psi(\mathbf{r_1})\rangle}{n(\mathbf{r_1})\cdots n(\mathbf{r_k})}, \tag{14}$$

and, by construction, $g^{(1)}(\mathbf{r_1}) = 1$. Then, by expanding the term $V_{eff}(\mathbf{r}' + \tau/2) - V_{eff}(\mathbf{r}' - \tau/2)$ in the integrand of Eq. (10) around $\tau = 0$ and using the Fourier integral theorem, we obtain the formal full expansion [14,15] to all orders in $\hbar$ of the Wigner equation in the generalized Hartree approximation [6]

$$\frac{\partial\mathcal{F}_{\mathcal{W}}}{\partial t} + \frac{p_k}{m}\frac{\partial\mathcal{F}_{\mathcal{W}}}{\partial x_k} = \sum_{l=0}^{\infty}\frac{(i\hbar/2)^{2l}}{(2l+1)!}\left[\frac{\partial^{2l+1}V_{eff}}{\partial x_{k_1}\cdots\partial x_{k_{2l+1}}}\right] \times \left[\frac{\partial^{2l+1}\mathcal{F}_{\mathcal{W}}}{\partial p_{k_1}\cdots\partial p_{k_{2l+1}}}\right], \tag{15}$$

where Einstein convention is used on the saturated indices $k, k_1, \ldots, k_{2l+1}$, and the effects of interactions are entirely contained in the definition of the effective potential $V_{eff}(\mathbf{r})$. We remark that if we consider only the first term in the sum of expression (13) (i.e., $L = 2$), then we obtain the usual Hartree approximation [16] with two-body interactions

$$V_{eff}(\mathbf{r}) = V(\mathbf{r}) + \int d^3r_1 n(\mathbf{r_1})V(\mathbf{r},\mathbf{r_1}), \tag{16}$$

while, by considering the remaining terms contained in Eq. (13) (i.e., for $L > 2$), in the expression of the effective potential we include other correction terms that are imputable to many-body interactions of higher order. Accordingly, by considering, for instance, a system of N electrons, this method provides the quantum Hartree equation [with the Coulomb potential $V(\mathbf{r},\mathbf{r_1}) = e^2/|\mathbf{r} - \mathbf{r_1}|$] written in the Wigner formalism, plus some corrections due to electron correlations. Analogously, in the case of a dilute gas of bosonic atoms, for $L = 2$ it is possible to approximate the two-body interactions by a delta function pseudopotential [17] assuming $V(\mathbf{r},\mathbf{r_1}) = c_1\delta(\mathbf{r} - \mathbf{r_1})$ with c_1 as the coupling constant between particles. Thus, by Eq. (16) we obtain, in the Hartree approximation, $V_{eff}(\mathbf{r}) = V(\mathbf{r}) + c_1 n(\mathbf{r})$. This procedure can be easily generalized to a Bose gas with many-body contact interactions [18] by setting $V(\mathbf{r_1},\mathbf{r_2},\ldots,\mathbf{r_k}) = c_{k-1}\Pi_{i=1}^{k-1}\delta(\mathbf{r_i} - \mathbf{r_{i+1}})$ for $\forall k \geq 2$. In this case we obtain

$$V_{eff}(\mathbf{r}) = V(\mathbf{r}) + \sum_{s=1}^{L-1}\frac{c_s}{s!}g^{(s)}(\underbrace{\mathbf{r},\ldots,\mathbf{r}}_{s\ \text{times}})[n(\mathbf{r})]^s, \tag{17}$$

and all nonlinear phenomena imputable to weak interactions between bosons can be expressed in terms of increasing powers of density, being $g^{(s)}(\mathbf{r},\ldots,\mathbf{r}) = \langle[\Psi^\dagger(\mathbf{r})]^s[\Psi(\mathbf{r})]^s\rangle/[n(\mathbf{r})]^s$ [19]. The advantage of this approach will be evident in the corresponding QHD system, since all closure relations imputable to the contact interactions can be *explicitly determined* as known polynomial functions of the macroscopic field variable $n(\mathbf{r})$ [20]. In this sense, the theory based on Eqs. (13)–(15) is a second major result of this work. Indeed, the present method provides the quantum Hartree approximation, written in the Wigner formalism, plus some corrections due to fermion and/or boson correlations. Finally, we remark that these results can be generalized by including explicitly the spin degrees of freedom. Equations (10) and (15) can be supplemented by other interaction terms to describe a variety of physical systems, including Fermi liquids [13], nonideal gases, and plasma [21].

Below, we develop the extended three-dimensional QHD model associated with Eq. (15) *to all orders* of $\hbar$. Following Ref. [4], by introducing the group velocity $u_i = p_i/m$, we define the mean velocity $v_i = n^{-1}\int d^3p u_i\mathcal{F}_{\mathcal{W}}$, the peculiar velocity $\tilde{u}_i = u_i - v_i$, and the quantity $\tilde{\varepsilon} = m\tilde{u}^2/2$. Then, we consider the set of traceless kinetic fields [22] $\tilde{\mathcal{M}}_A = \{\tilde{\varepsilon}^s, \tilde{\varepsilon}^s\tilde{u}_{i_1}, \ldots, \tilde{\varepsilon}^s\tilde{u}_{\langle i_1}\tilde{u}_{i_2}\cdots\tilde{u}_{i_r\rangle}\}$ and the corresponding set of *central moments* $M_A(\mathbf{r},t) = \{M_{(s)}, M_{(s)|i_1}, \ldots, M_{(s)|\langle i_1\cdots i_r\rangle}\}$ where, by construction, it is $M_{(0)|i_1} = 0$ and

$$M_{(s)|\langle i_1 i_2\cdots i_r\rangle} = \int d^3p\,\tilde{\varepsilon}^s\tilde{u}_{\langle i_1}\tilde{u}_{i_2}\cdots\tilde{u}_{i_r\rangle}\mathcal{F}_{\mathcal{W}}, \tag{18}$$

with $s = 0, 1, \ldots, \mathcal{N}$ and $r = 1, 2, \ldots, M$. In particular, by using a finite but arbitrary number of scalar and vectorial kinetic fields $\tilde{\mathcal{M}}_A = \{\tilde{\varepsilon}^s, \tilde{\varepsilon}^s\tilde{u}_i\}$ we obtain in correspondence the set of scalar and vectorial central moments $M_A = \{M_{(s)}, M_{(s)|i}\}$, with $s = 0, \ldots, \mathcal{N}$. Accordingly, for $\mathcal{N} = 0$, as set of macroscopic variables we get the *numerical density* $n = M_{(0)}$ and the *velocity* v_i. For $\mathcal{N} = 1$, we get in addition $M_{(1)}$ and $M_{(1)|i}$, which admit a direct physical interpretation being $M_{(1)} = 3/2\ P$ and $M_{(1)|i} = q_i$, respectively, the *internal energy density* (with P as the pressure) and the *heat flux density*. By contrast, for $\mathcal{N} > 1$, as macroscopic variables, we consider also some scalar and vectorial moments of higher order. Multiplying Eq. (15) by $\tilde{\mathcal{M}}_A$, integrating over $\mathbf{p}$ we exactly determine, to all orders of $\hbar$, the corresponding set of QHD equations,

$$\dot{n} + n\frac{\partial v_k}{\partial x_k} = 0, \tag{19}$$

$$\dot{v}_i + \frac{1}{n}\frac{\partial M_{(0)|ik}}{\partial x_k} + \frac{1}{m}\frac{\partial V_{eff}}{\partial x_i} = 0, \tag{20}$$

$$\begin{aligned}\dot{M}_{(s)} &+ M_{(s)}\frac{\partial v_k}{\partial x_k} + smM_{(s-1)|ik}\frac{\partial v_i}{\partial x_k} + \frac{\partial M_{(s)|k}}{\partial x_k} - s\frac{m}{n}M_{(s-1)|i}\frac{\partial M_{(0)|ik}}{\partial x_k}\\ &= -\sum_{l=1}^{s-1}\frac{(i\hbar/2)^{2l}}{(2l+1)!}\sum_{r=q}^{l}B_{sl}^{(0)r}\Bigg\{\frac{\partial^{2r}}{\partial x_{\beta_1}^2\cdots\partial x_{\beta_r}^2}\frac{\partial^{2(l-r)+1}V_{eff}}{\partial x_{k_1}\cdots\partial x_{k_{2(l-r)+1}}}M_{(s+r-2l-1)|\langle k_1\cdots k_{2(l-r)+1}\rangle}\\ &\quad + \sum_{j=1}^{l-r}A_{lr}^{(0)j}\frac{\partial^{2(r+j)}}{\partial x_{\beta_1}^2\cdots\partial x_{\beta_{r+j}}^2}\frac{\partial^{2(l-r-j)+1}V_{eff}}{\partial x_{k_1}\cdots\partial x_{k_{2(l-r-j)+1}}}M_{(s+r+j-2l-1)|\langle k_1\cdots k_{2(l-r-j)+1}\rangle}\Bigg\},\end{aligned} \tag{21}$$

$$\begin{aligned}\dot{M}_{(s)|i} &+ M_{(s)|i}\frac{\partial v_k}{\partial x_k} + smM_{(s-1)|ipk}\frac{\partial v_p}{\partial x_k} + M_{(s)|k}\frac{\partial v_i}{\partial x_k} - \frac{M_{(s)}}{n}\frac{\partial M_{(0)|ik}}{\partial x_k} - sm\frac{M_{(s-1)|ip}}{n}\frac{\partial M_{(0)|pk}}{\partial x_k} + \frac{\partial M_{(s)|ik}}{\partial x_k}\\ &= -\sum_{l=1}^{s}\frac{(i\hbar/2)^{2l}}{(2l+1)!}\frac{\partial^{2l+1}V_{eff}}{\partial x_{k_1}\cdots\partial x_{k_{2l+1}}}\sum_{r=q}^{l+1}B_{sl}^{(1)r}\Bigg\{M_{(s+r-2l-1)|(\langle k_1\cdots k_{2(l-r)+2}\rangle}\delta_{k_{2(l-r)+3}k_{2(l-r)+4}}\cdots\delta_{k_{2l+1}i)}\\ &\quad + \sum_{j=1}^{l-r+1}A_{lr}^{(1)j}M_{(s+r+j-2l-1)|(\langle k_1\cdots k_{2(l-r-j)+2}\rangle}\delta_{k_{2(l-r-j)+3}k_{2(l-r-j)+4}}\cdots\delta_{k_{2l+1}i)}\Bigg\}\quad \text{with } s=1,\ldots,\mathcal{N},\end{aligned} \tag{22}$$

being the index $q=\max\{0,(2l+1-s)\}$ and the coefficients $\{B_{sl}^{(p)r},A_{lr}^{(p)j}\}$ (for $p=0,1$) expressed by the relations

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

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

We remark that by considering the complete expansion in Eq. (15) it follows that in each QHD scalar and vectorial equation only a finite number of terms in powers of $\hbar^2$ remain. The set of equations (19)–(22), which for $\hbar \to 0$ recovers the classical form of extended thermodynamics [4,23], is a third major result of the work. This set contains unknown constitutive functions that, through Eq. (18), are represented by the central moments of higher order with respect to the scalar and vectorial macroscopic variables $\{M_{(s)},M_{(s)|i}\}$.

In general, the closure problem of a set of balance equations is tackled using the previous QMEP formalism. Thus, for a given number of moments M_A, we consider a consistent expansion around $\hbar$ of the Wigner function. In this way we separate classical from quantum dynamics, and we obtain order by order correction terms. In particular, by using the Moyal formalism one can prove [14,24] that the Wigner function, and hence the central moments, can be expanded in even power of $\hbar$ as

$$\mathcal{F}_{\mathcal{W}} = \sum_{k=0}^{\infty}\hbar^{2k}\mathcal{F}_{\mathcal{W}}^{(2k)}, \quad M_A = \sum_{k=0}^{\infty}\hbar^{2k}M_A^{(2k)}. \tag{23}$$

With this approach, the dynamics of the system is described by resolving, order by order, a closed QHD set of balance equations for the moments $\{M_A(\mathbf{r},t)\}$. To this end, the Lagrange multipliers λ_A must be determined by inverting, order by order, the constraints

$$M_A = (2\pi\hbar)^{-3}\int d^3p\,\tilde{\mathcal{M}}_A\mathcal{W}(\hat{\varrho}[\lambda_B(\mathbf{r},t),\tilde{\mathcal{M}}_B]). \tag{24}$$

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

$$\lambda_A = \lambda_A^{(0)} + \sum_{k=1}^{\infty}\hbar^{2k}\lambda_A^{(2k)}. \tag{25}$$

With these assumptions, and using Eqs. (8) and (9), we succeed in determining the following expression for $\mathcal{F}_{\mathcal{W}}$:

$$\mathcal{F}_{\mathcal{W}} = \frac{\tilde{y}}{e^{\Pi} \pm 1}\left\{1 + \sum_{r=1}^{\infty} \hbar^{2r} P_{2r}^{\pm}\right\}, \tag{26}$$

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

Equation (26) is a fourth major result of the work. The Lagrange multipliers can be obtained, order by order, as solutions of Eq. (24). Furthermore, the central moments M_A must satisfy the QHD system of equations (19)–(22) to the same prefixed order in powers of $\hbar$. From the knowledge of the Lagrange multipliers, both the Wigner function and the constitutive functions can be determined explicitly.

III. SOME EXAMPLES OF CLOSED QHD SYSTEMS

As relevant examples of the previous approach we use only the first two terms of Eq. (26) and decompose the Lagrange multipliers in the equilibrium and nonequilibrium local parts $\Pi=\alpha+\beta\tilde{\varepsilon}+\Sigma\Lambda_A\tilde{\mathcal{M}}_A$, with $\{\alpha(\mathbf{r},t),\beta(\mathbf{r},t)\}$ being the nonvanishing Lagrange multipliers of local equilibrium and $\Lambda_A(\mathbf{r},t)$ being that of nonequilibrium. In this way, we consider an expansion up to first order in the deviations from the local equilibrium configuration $\mathcal{F}_{\mathcal{W}}|_E$,

$$\mathcal{F}_{\mathcal{W}} \approx \mathcal{F}_{\mathcal{W}}|_E + \sum_{A=1}^{N}\left[\frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial \Lambda_A}\right]_E \Lambda_A,$$

and obtain the approximate relations

$$\mathcal{F}_{\mathcal{W}}|_E \approx \tilde{y}[L_{(0)}^{\pm} + \hbar^2 P_2^{\pm(0)}], \tag{27}$$

$$\mathcal{F}_{\mathcal{W}}|_{NE} \approx \tilde{y}[L_{(1)}^{\pm} + \hbar^2 P_2^{\pm(1)}]\sum_{l=0}^{\mathcal{N}}\{\Lambda_{(l)}\tilde{\varepsilon}^l + \Lambda_{(l)|i}\tilde{\varepsilon}^l\tilde{u}_i\}, \tag{28}$$

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

$$L_{(n)}^{\pm} = \frac{d^n}{d\alpha^n}\left\{\frac{1}{e^{\alpha+\beta\tilde{\varepsilon}} \pm 1}\right\}. \tag{29}$$

If, for the sake of simplicity, we assume that nonlocal effects are imputable only to the spatial derivatives of density n, then the quantum correction terms $P_2^{\pm(r)}$ (with $r=0,1$) are expressed in the form

$$P_2^{\pm(r)} = \frac{1}{12m}\frac{1}{k_BT}\Bigg\{[L_{(3+r)}^{\pm}Q^{(1)} + 9L_{(2+r)}^{\pm}Q^{(2)}] + \frac{m}{k_BT}L_{(3+r)}^{\pm}[Q^{(2)}\tilde{u}^2 + Q_{\langle ij\rangle}\tilde{u}_{\langle i}\tilde{u}_{j\rangle}]\Bigg\} + \mathcal{O}(\hbar^2), \tag{30}$$

where T is an effective temperature and the nonlocal quantities $\{Q^{(k)},Q_{\langle ij\rangle}\}$ are explicitly reported in Eqs. (A3)–(A5) of Appendix A. With this approach, the Lagrange multipliers are determined by inverting the relations

$$M_A + \mathcal{O}(\hbar^4) = \int d^3p\,\tilde{\mathcal{M}}_A\mathcal{F}_{\mathcal{W}}. \tag{31}$$

where, in the course of computation, we assume that the quantities M_A satisfy the QHD system of equations (19)–(22) up to terms of order $\hbar^2$. Consequently, if we know the Lagrange multipliers, then we determine all the closure relations for the system, up to first-order quantum correction. In particular, by assuming for $\beta=(k_BT)^{-1}$ the Lagrange multiplier of local equilibrium α is obtained by inverting the constraint,

$$n + \mathcal{O}(\hbar^4) = \int d^3p\,\mathcal{F}_{\mathcal{W}}|_E, \tag{32}$$

and solving the following relation with respect to α:

$$I_2^{\pm}(\alpha) = \gamma\frac{n}{T^{3/2}}\left\{1 + \frac{\hbar^2}{32m}\frac{1}{k_BT}\left[\frac{I_{-4}^{\pm}}{I_2^{\pm}}Q^{(1)} + 4\frac{I_{-2}^{\pm}}{I_2^{\pm}}Q^{(2)}\right]\right\} + \mathcal{O}(\hbar^4), \tag{33}$$

where $\gamma^{-1}=[4(2\tilde{s}+1)/\sqrt{\pi}](mk_B/2\pi\hbar^2)^{3/2}$ and $I_n^{\pm}(\alpha)$ are the Fermi and Bose integral functions reported explicitly in Appendix A. Analogously, using the remaining local equilibrium relation

$$P + \mathcal{O}(\hbar^4) = \frac{2}{3}\int d^3p\,\tilde{\varepsilon}\mathcal{F}_{\mathcal{W}}|_E, \tag{34}$$

we obtain the generalized expression for the pressure P and consequently the quantum equation of state that represents a *differential constraint* [25] for the QHD system,

$$P = \frac{2}{3}n\frac{I_4^{\pm}}{I_2^{\pm}}\Bigg\{k_BT + \frac{\hbar^2}{8m}\Bigg[\frac{1}{4}\left(\frac{I_{-2}^{\pm}}{I_4^{\pm}} + \frac{I_{-4}^{\pm}}{I_2^{\pm}}\right)Q^{(1)} + \left(2\frac{I_0^{\pm}}{I_4^{\pm}} + \frac{I_{-2}^{\pm}}{I_2^{\pm}}\right)Q^{(2)}\Bigg]\Bigg\} + \mathcal{O}(\hbar^4), \tag{35}$$

where, for arbitrary values of α, all statistic information is contained in the Fermi and Bose integral functions $I_n^{\pm}(\alpha)$, while the nonlocality is expressed by the differential terms $\{Q^{(k)},Q_{\langle ij\rangle}\}$. We remark that every set of closed QHD equations must be supplemented by differential constraints (33) and (35). In general, these differential relations must be solved numerically, step by step with the closed QHD system. In this way it is possible to determine numerically both the Lagrange multiplier α (or, equivalently, the chemical potential $\mu=-\alpha k_BT$) and the pressure P as numerical functions of variables n and T. However, it is possible to show that, by introducing the usual Bohm quantum potential $Q_B=-(\hbar^2/2m\sqrt{n})\Delta\sqrt{n}$, some simplified analytical cases can be analyzed.

Completely nondegenerate gases. For $\alpha \gg 1$ both the Bose and Fermi statistics tend to Boltzmann statistic and we determine the results obtained for the quantum Boltzmann gas (see Appendix B). In particular, by using relations (33) and (35) we recover the well-known expressions for the quantum chemical potential [26] and for the quantum pressure [27,28],

$$\mu = k_BT\ln\left[\frac{4\gamma}{\sqrt{\pi}}\frac{n}{T^{3/2}}\right] + \frac{Q_B}{3} + \mathcal{O}(\hbar^4), \tag{36}$$

$$P = nk_BT - \frac{\hbar^2}{36}\frac{n}{m}\frac{\partial^2\ln n}{\partial x_r\,\partial x_r} + \mathcal{O}(\hbar^4). \tag{37}$$

Weakly degenerate Fermi and Bose gases. For $\alpha > 1$ we describe the Fermi and Bose statistics of a weakly degenerate gas by considering the first two terms of a suitable expansion in series for the integral functions $I_n^{\pm}(\alpha)$. Accordingly, we obtain (see Appendix B) the statistical corrections for both the quantum chemical potential and the quantum pressure in the case of a *weakly degenerate* gas,

$$\mu = k_B T \ln\left[\left(1 \pm \frac{\chi^{(0)}}{2^{3/2}}\right)\chi^{(0)}\right] + \frac{1}{3}\left(Q_B \pm \frac{\chi^{(0)}}{2^{3/2}} Q_C\right) + \mathcal{O}(\hbar^4), \tag{38}$$

$$P = n k_B T\left(1 \pm \frac{\chi^{(0)}}{2^{5/2}}\right) - \frac{\hbar^2}{36}\frac{n}{m}\left[\left(1 \mp \frac{3}{2^{3/2}}\chi^{(0)}\right)\frac{\partial^2 \ln n}{\partial x_r \partial x_r} \mp \frac{7}{2^{5/2}}\chi^{(0)}\left(\frac{\partial \ln n}{\partial x_r}\right)^2\right] + \mathcal{O}(\hbar^4), \tag{39}$$

where $\chi^{(0)} = (4\gamma/\sqrt{\pi})(n/T^{3/2}) \ll 1$ and

$$Q_C = \frac{\hbar^2}{4m}\left\{\frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \left(\frac{\partial \ln n}{\partial x_r}\right)^2\right\}. \tag{40}$$

Completely degenerate Fermi gases. When $T \to 0$, the degeneracy of a Fermi gas becomes complete. In this case, the Fermi integral functions $I_n^{+}(\alpha)$ assume a simplified form and we obtain (see Appendix B) the following relations for both the quantum chemical potential and the quantum pressure:

$$\mu = \frac{5}{2}\nu_F n^{2/3} + \frac{Q_B}{9} + \mathcal{O}(\hbar^4), \tag{41}$$

$$P = \nu_F n^{5/3} + \frac{\hbar^2}{36}\frac{n}{m}\left\{\frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \frac{4}{3}\left(\frac{\partial \ln n}{\partial x_r}\right)^2\right\} + \mathcal{O}(\hbar^4), \tag{42}$$

where $\nu_F = (\hbar^2/5m)[6\pi^2/(2\tilde{s}+1)]^{2/3}$.

Strongly degenerate Fermi gases. For $-\alpha \gg 1$ and $T > 0$ we consider the Fermi statistics for a strongly degenerate gas and we can determine the statistical corrections (see Appendix B) for both the quantum chemical potential and the quantum pressure,

$$\mu = \mu^{(0)}\left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\mu^{(0)}}\right)^2\right] + \frac{1}{9}\left[Q_B + \frac{\pi^2}{12}\left(\frac{k_B T}{\mu^{(0)}}\right)^2 \tilde{Q}_C\right] + \mathcal{O}(\hbar^4), \tag{43}$$

$$P = \nu_F n^{5/3}\left[1 + \frac{5}{12}\pi^2\left(\frac{k_B T}{\mu^{(0)}}\right)^2\right] + \frac{\hbar^2}{36}\frac{n}{m}\left\{\left[1 - \frac{\pi^2}{3}\left(\frac{k_B T}{\mu^{(0)}}\right)^2\right]\frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \frac{4}{3}\left(\frac{\partial \ln n}{\partial x_r}\right)^2\right\} + \mathcal{O}(\hbar^4), \tag{44}$$

where $\mu^{(0)} = (5\nu_F/2)n^{2/3}$ and

$$\tilde{Q}_C = -\frac{\hbar^2}{6m}\left\{6\frac{\partial^2 \ln n}{\partial x_r \partial x_r} - \left(\frac{\partial \ln n}{\partial x_r}\right)^2\right\}. \tag{45}$$

Finally, we use the present approach to obtain some examples of closed QHD systems. Accordingly, by considering the QHD equations (19)–(22) for $\mathcal{N}=0,1$, we determine the following closed systems.

A. Quantum drift-diffusion model

For $\mathcal{N}=0$ we obtain the usual quantum drift-diffusion model with the balance equations (19) and (20) for the macroscopic variables $\{n, v_i\}$,

$$\frac{\partial n}{\partial t} + \frac{\partial n v_k}{\partial x_k} = 0, \tag{46}$$

$$\frac{\partial v_i}{\partial t} + v_k \frac{\partial v_i}{\partial x_k} + \frac{1}{n}\frac{\partial M_{(0)|ik}}{\partial x_k} + \frac{1}{m}\frac{\partial V_{eff}}{\partial x_i} = 0. \tag{47}$$

In this case: (i) The effective temperature T_0 is necessarily constant. (ii) The parameters $\beta = (k_B T_0)^{-1}$, α, and P are expressed by using the general differential relations (33) and (35) with $T = T_0$. (iii) The pressure P and the *stress deviator* [29] $M_{(0)|\langle ik\rangle}$ are independent constitutive quantities being

$$M_{(0)|ik} = M_{(0)|\langle ik\rangle} + \frac{P}{m}\delta_{ik}, \tag{48}$$

and the general closure relation for the traceless tensor $M_{(0)|\langle ik\rangle} = \int d^3p\, \tilde{u}_{\langle i}\tilde{u}_{k\rangle}\mathcal{F}_{\mathcal{W}}$ is determined by inserting in its kinetic definition the relations (27)–(30). Thus, we obtain the general expression

$$M_{(0)|\langle ik\rangle} = -\frac{\hbar^2}{12}\frac{n}{m^2}\frac{I_0^{\pm}}{I_2^{\pm}}Q_{\langle ik\rangle} + \mathcal{O}(\hbar^4), \tag{49}$$

where the nonlocal term $Q_{\langle ik\rangle}$ is given by Eq. (A5) in Appendix A. In this way the system of equations (46) and (47) is closed. In particular, we consider the following different analytical cases for the explicit closure relations.

1. Completely nondegenerate Fermi and Bose gases

In this case the pressure P is given by Eq. (37) (with $T = T_0$), while for the traceless tensor in Eq. (49) it is (see Appendix B)

$$M_{(0)|\langle ik\rangle} = -\frac{\hbar^2}{12}\frac{n}{m^2}\frac{\partial^2 \ln n}{\partial x_{\langle i}\partial x_{k\rangle}} + \mathcal{O}(\hbar^4). \tag{50}$$

Thus, by Eq. (48) we obtain the known *closure relation* [27,28] for the stress tensor [29]

$$M_{(0)|ik} = \frac{n}{m}\left\{k_B T_0 \delta_{ik} - \frac{\hbar^2}{12m}\frac{\partial^2 \ln n}{\partial x_i \partial x_k}\right\} + \mathcal{O}(\hbar^4) \tag{51}$$

and using identity (A9) we recover the well-known expression [27] for nondegenerate gases

$$\frac{\partial M_{(0)|ik}}{\partial x_k} = \frac{1}{m}\left\{k_B T_0 \frac{\partial n}{\partial x_i} + \frac{n}{3}\frac{\partial Q_B}{\partial x_i}\right\} + \mathcal{O}(\hbar^4), \tag{52}$$

in terms of the Bohm potential.

2. Weakly degenerate Fermi and Bose gases

In this case, the pressure is expressed by Eq. (39) (with $T=T_0$), while by using relation (49) (see Appendix B) we obtain the statistical correction

$$M_{(0)|\langle ik\rangle} = -\frac{\hbar^2}{12}\frac{n}{m^2}\left\{\frac{\partial^2 \ln n}{\partial x_{\langle i}\partial x_{k\rangle}} \pm \frac{\chi^{(0)}}{2^{3/2}}\frac{\partial \ln n}{\partial x_{\langle i}}\frac{\partial \ln n}{\partial x_{k\rangle}}\right\} + \mathcal{O}(\hbar^4). \tag{53}$$

Thus, by Eq. (48) we determine the explicit closure relation for $M_{(0)|ik}$. In this context, it is easy to verify that the spatial derivative of the stress tensor can be rewritten in the simplified form

$$\frac{\partial M_{(0)|ik}}{\partial x_k} = \frac{1}{m}\left\{k_B T_0 \frac{\partial}{\partial x_i}\left[n\left(1 \pm \frac{\chi^{(0)}}{2^{5/2}}\right)\right] + \frac{n}{3}\frac{\partial}{\partial x_i}\left[Q_B \pm \frac{\chi^{(0)}}{2^{3/2}}Q_C\right]\right\} + \mathcal{O}(\hbar^4), \tag{54}$$

and, as a consequence, we obtain the following explicit statistical quantum correction:

$$\frac{\partial M_{(0)|ik}}{\partial x_k} = \frac{k_B T_0}{m}\frac{\partial n}{\partial x_i} + \frac{n}{3m}\frac{\partial Q_B}{\partial x_i} \pm \frac{2\gamma}{\sqrt{2\pi}}\frac{n}{T_0^{3/2}}\left[\frac{k_B T_0}{m}\frac{\partial n}{\partial x_i} + \frac{\hbar^2}{12m^2}\frac{\partial \Delta n}{\partial x_i}\right] + \mathcal{O}(\hbar^4) \tag{55}$$

for the system of equations (46) and (47).

3. Completely degenerate Fermi gases

In this case the pressure P is given by Eq. (42) while, for the traceless tensor of Eq. (49), it is (see Appendix B)

$$M_{(0)|\langle ik\rangle} = -\frac{\hbar^2}{12}\frac{n}{m^2}\left\{\frac{\partial^2 \ln n}{\partial x_{\langle i}\partial x_{k\rangle}} + \frac{2}{3}\frac{\partial \ln n}{\partial x_{\langle i}}\frac{\partial \ln n}{\partial x_{k\rangle}}\right\} + \mathcal{O}(\hbar^4). \tag{56}$$

Thus, by Eq. (48) we obtain the explicit closure relation for the stress tensor,

$$M_{(0)|ik} = \frac{\nu_F}{m}n^{5/3}\delta_{ik} - \frac{\hbar^2}{36}\frac{n}{m^2}\left\{3\frac{\partial^2 \ln n}{\partial x_i\,\partial x_k} + 2\frac{\partial \ln n}{\partial x_i}\frac{\partial \ln n}{\partial x_k} - 2\left[\left(\frac{\partial \ln n}{\partial x_r}\right)^2 + \frac{\partial^2 \ln n}{\partial x_r\,\partial x_r}\right]\delta_{ik}\right\} + \mathcal{O}(\hbar^4), \tag{57}$$

and using identities (A8)–(A10) we obtain the simplified relation, for a *completely degenerate* Fermi gas,

$$\frac{\partial M_{(0)|ik}}{\partial x_k} = \frac{1}{m}\left\{\frac{5}{3}\nu_F n^{2/3}\frac{\partial n}{\partial x_i} + \frac{n}{9}\frac{\partial Q_B}{\partial x_i}\right\} + \mathcal{O}(\hbar^4). \tag{58}$$

4. Strongly degenerate Fermi gases

In strong degenerate conditions, the pressure is expressed by Eq. (44) (with $T=T_0$) while, by using relation (49) (see Appendix B), we obtain the statistical correction for the traceless tensor,

$$M_{(0)|\langle ik\rangle} = -\frac{\hbar^2}{12}\frac{n}{m^2}\left\{\frac{\partial^2 \ln n}{\partial x_{\langle i}\partial x_{k\rangle}} + \frac{2}{3}\left[1 - \frac{\pi^2}{6}\left(\frac{k_B T_0}{\mu^{(0)}}\right)^2\right]\frac{\partial \ln n}{\partial x_{\langle i}}\frac{\partial \ln n}{\partial x_{k\rangle}}\right\} + \mathcal{O}(\hbar^4). \tag{59}$$

As a consequence, by using Eq. (48) we obtain the expression for the stress tensor $M_{(0)|ik}$ and the system of equations (46) and (47) is explicitly closed. Also in this case, it is possible to verify that the spatial derivative of the stress tensor can be rewritten in the simplified form

$$\frac{\partial M_{(0)|ik}}{\partial x_k} = \frac{1}{m}\left(\nu_F\frac{\partial}{\partial x_i}\left\{n^{5/3}\left[1 + \frac{5\pi^2}{12}\left(\frac{k_B T_0}{\mu^{(0)}}\right)^2\right]\right\} + \frac{n}{9}\frac{\partial}{\partial x_i}\left[Q_B + \frac{\pi^2}{12}\left(\frac{k_B T_0}{\mu^{(0)}}\right)^2\tilde{Q}_C\right]\right) + \mathcal{O}(\hbar^4). \tag{60}$$

In conclusion, by indicating with $\{\mu^{(c)}, P^{(c)}\}$ and $\{\mu^{(q)}, P^{(q)}\}$, respectively, the classical and the quantum parts of the chemical potential and pressure, we remark that all relations (52), (54), (58), and (60) will be expressed by means of the *general closure property*

$$\frac{\partial M_{(0)|ik}}{\partial x_k} = \frac{1}{m}\left\{\frac{\partial P^{(c)}}{\partial x_i} + n\frac{\partial \mu^{(q)}}{\partial x_i}\right\} + \mathcal{O}(\hbar^4) \tag{61}$$

for the quantum drift-diffusion system in Eqs. (46) and (47).

B. QHD model for the moments $\{n, v_i, P, q_i\}$

For $\mathcal{N}=1$ we consider the QHD system in Eqs. (22)–(25) for the macroscopic variables $\{n, v_i, P, q_i\}$, which admits for a direct physical interpretation the *pressure* $P=2/3\,M_{(1)}$ and the heat flux density $q_i=M_{(1)|i}$. Accordingly, we find the balance equations

$$\frac{\partial n}{\partial t} + \frac{\partial n v_k}{\partial x_k} = 0, \tag{62}$$

$$\frac{\partial v_i}{\partial t} + v_k\frac{\partial v_i}{\partial x_k} + \frac{1}{n}\frac{\partial}{\partial x_k}\left\{M_{(0)|\langle ik\rangle} + \frac{P}{m}\delta_{ik}\right\} + \frac{1}{m}\frac{\partial V_{eff}}{\partial x_i} = 0, \tag{63}$$

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial x_k}\left\{P v_k + \frac{2}{3}q_k\right\} + \frac{2}{3}P\frac{\partial v_k}{\partial x_k} + \frac{2}{3}m M_{(0)|\langle ik\rangle}\frac{\partial v_i}{\partial x_k} = 0, \tag{64}$$

$$\frac{\partial q_i}{\partial t} + \frac{\partial}{\partial x_k}\left\{q_i v_k + M_{(1)|\langle ik\rangle} + \frac{2}{3}\frac{1}{m}M_{(2)}\delta_{ik}\right\} + m M_{(0)|\langle ijk\rangle}\frac{\partial v_j}{\partial x_k} - \frac{5}{2}\frac{P}{n}\frac{\partial}{\partial x_k}\left\{M_{(0)|\langle ik\rangle} + \frac{P}{m}\delta_{ik}\right\} - \frac{m}{n}M_{(0)|\langle ij\rangle}\frac{\partial}{\partial x_k}\left\{M_{(0)|\langle jk\rangle} + \frac{P}{m}\delta_{jk}\right\} + \frac{2}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} = \frac{\hbar^2}{8m^2}n\frac{\partial^3 V_{eff}}{\partial x_k\,\partial x_k\,\partial x_i}. \tag{65}$$

In this case: (i) we have the effective local temperature $T(\mathbf{r},t)$ with $\beta=(k_BT)^{-1}$, (ii) the system in Eqs. (62)–(65) must be supplemented by the differential constraints in Eqs. (33) and (35) to determine α and P, and (iii) the nonequilibrium quantum Lagrange multipliers $\{\Lambda_{(l)},\Lambda_{(l)|i}\}$ (for $l=0,1$) can be determined by inverting relations (31) evaluated in nonequilibrium conditions. Thus, if we know the Lagrange multipliers, then we determine all closure relations for the system, up to the first quantum correction. In this case, we report explicitly only the constitutive functions $H_A=\{M_{(0)|\langle ik\rangle},M_{(1)|\langle ik\rangle},M_{(0)|\langle ijk\rangle},M_{(2)}\}$, which will be given through the general relations

$$M_{(0)|\langle ik\rangle}=-\frac{1}{12}\frac{\hbar^2}{m^2}n\frac{I_0^{\pm}}{I_2^{\pm}}Q_{\langle ik\rangle}+\mathcal{O}(\hbar^4), \tag{66}$$

$$M_{(1)|\langle ik\rangle}=-\frac{7}{12}\frac{\hbar^2}{m^2}nk_BTQ_{\langle ik\rangle}+\mathcal{O}(\hbar^4), \tag{67}$$

$$M_{(0)|\langle ijk\rangle}=\frac{3}{4}\frac{\hbar^2}{m^2}\frac{\Phi}{k_BT}q_{\langle i}Q_{\langle jk\rangle\rangle}+\mathcal{O}(\hbar^4), \tag{68}$$

$$M_{(2)}=n\frac{I_6^{\pm}}{I_2^{\pm}}(k_BT)^2\left\{1+\frac{\hbar^2}{12m}\frac{1}{k_BT}[\zeta_1Q^{(1)}+\zeta_2Q^{(2)}]\right\}+\mathcal{O}(\hbar^4), \tag{69}$$

where the coefficients $\{\Phi,\zeta_1,\zeta_2\}$ are reported explicitly in Eqs. (A6) and (A7) of Appendix A. We remark that the closure relations (66)–(69) are valid for arbitrary values of α being expressed in terms of Fermi and Bose integral functions. Also in this case, it is possible to explore the different analytical cases reported in the previous sections. However, for the sake of simplicity we analyze explicitly only the results obtained in the framework of the Boltzmann statistic by reporting the following simplified closure relations for a completely nondegenerate gas:

$$M_{(0)|\langle ik\rangle}=-\frac{1}{12}\frac{\hbar^2}{m^2}n\frac{\partial^2\ln n}{\partial x_{\langle i}\,\partial x_{k\rangle}}+\mathcal{O}(\hbar^4), \tag{70}$$

$$M_{(1)|\langle ik\rangle}=-\frac{7}{24}\frac{\hbar^2}{m^2}nk_BT\frac{\partial^2\ln n}{\partial x_{\langle i}\,\partial x_{k\rangle}}+\mathcal{O}(\hbar^4), \tag{71}$$

$$M_{(0)|\langle ijk\rangle}=-\frac{1}{5}\frac{\hbar^2}{m^2}\frac{1}{k_BT}q_{\langle i}\frac{\partial^2\ln n}{\partial x_{\langle j}\,\partial x_{k\rangle\rangle}}+\mathcal{O}(\hbar^4), \tag{72}$$

$$M_{(2)}=\frac{15}{4}n(k_BT)^2\left\{1-\frac{\hbar^2}{18m}\frac{1}{k_BT}\frac{\partial^2\ln n}{\partial x_k\,\partial x_k}\right\}+\mathcal{O}(\hbar^4). \tag{73}$$

IV. CONCLUSION

The quantum maximum entropy principle is proposed here as a rigorous procedure that should be employed when it becomes necessary to treat systems in partially specified quantum-mechanical states. By considering the reduced density matrix, within a second-quantized formalism, we have described a many-body model for identical particles. In this respect we have shown that (i) using the general definition in Eqs. (8) and (9) we have incorporated the indistinguishability principle of a system of identical particles. Thus, by introducing a QMEP, in nonequilibrium conditions we have formulated a nonlocal theory that contains implicitly the Fermi and Bose statistics, a result which was left open since the Wigner seminal papers [14,24]. (ii) We have determined a generalized Wigner equation where the effects of interactions are entirely contained in the definition of the effective potential in Eq. (13). In this way we have recovered the quantum Hartree approximation, written in the Wigner formalism, plus some corrections due to fermion and/or boson correlations. (iii) We have developed to all orders in powers of $\hbar$ a quantum closure procedure for the corresponding QHD system. As simple examples we have reported explicitly, in the cases $\mathcal{N}=0,1$, the closure relations evaluated up to the first quantum approximation. In particular, in the framework of Boltzmann statistics, we have recovered the well-known expression for the quantum chemical potential, for the quantum pressure, and for the quantum closure scheme in the case of the standard drift-diffusion model. (iv) When $\hbar\rightarrow0$ we recover the expressions $\lambda_A^{(0)}=\lambda_A^{(0)}(M_B^{(0)})$ and $\mathcal{F}_{\mathcal{W}}^{(0)}$ obtained in the framework of classical MEP approach [4] for a fermion or boson system. In closing, we remark that this approach can be further generalized to develop a nonlocal theory for the fractional statistics. In this case, the entropy of the system should be expressed in terms of the *statistical weight* introduced by Wu [30] and the QMEP should be developed in terms of the reduced density matrix for particles obeying fractional exclusion statistics.

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APPENDIX A

We define the Fermi and the Bose integral functions

$$I_n^{\pm}(\alpha)=\int_0^{+\infty}\frac{x^n}{\exp(\alpha+x^2)\pm1}dx, \tag{A1}$$

satisfying the differentiation property

$$\frac{d^rI_n^{\pm}(\alpha)}{d\alpha^r}=(-1)^r\frac{\Gamma\left(\frac{n+1}{2}\right)}{\Gamma\left(\frac{n+1}{2}-r\right)}I_{n-2r}^{\pm}(\alpha), \tag{A2}$$

where this relation cannot be necessarily restricted to positive values of n; thus, all function $I_n^{\pm}(\alpha)$ with negative values of n are defined by means of Eq. (A2). The nonlocal terms $\{Q^{(1)},Q^{(2)},Q_{\langle ij\rangle}\}$ are expressed by

$$Q^{(1)} = -2\left(\frac{I_2^\pm}{I_0^\pm}\right)^2\left(\frac{\partial \ln n}{\partial x_k}\right)^2 + \mathcal{O}(\hbar^2), \tag{A3}$$

$$Q^{(2)} = \frac{1}{3}\frac{I_2^\mp}{I_0^\pm}\left\{\left[1 + \frac{I_2^\pm}{I_0^\pm}\frac{I_{-2}^\pm}{I_0^\pm}\right]\left(\frac{\partial \ln n}{\partial x_k}\right)^2 + \frac{\partial^2 \ln n}{\partial x_k\,\partial x_k}\right\} + \mathcal{O}(\hbar^2), \tag{A4}$$

$$Q_{\langle ij\rangle} = \frac{I_2^\pm}{I_0^\pm}\left\{\left[1 + \frac{I_2^\pm}{I_0^\pm}\frac{I_{-2}^\pm}{I_0^\pm}\right]\frac{\partial \ln n}{\partial x_{\langle i}}\frac{\partial \ln n}{\partial x_{j\rangle}} + \frac{\partial^2 \ln n}{\partial x_{\langle i}\partial x_{j\rangle}}\right\} + \mathcal{O}(\hbar^2). \tag{A5}$$

The coefficients $\{\Phi,\zeta_1,\zeta_2\}$, contained in the constitutive functions (68) and (69), are given by the relations

$$\Phi = \frac{27(I_2^\pm)^2 - 5I_0^\pm I_4^\pm}{25(I_4^\pm)^2 - 21 I_2^\pm I_6^\pm}, \tag{A6}$$

$$\zeta_1 = \frac{3}{8}\left[\frac{I_{-4}^\pm}{I_2^\pm} - 5\frac{I_0^\pm}{I_6^\pm}\right], \qquad \zeta_2 = \frac{3}{2}\left[\frac{I_{-2}^\pm}{I_2^\pm} + 5\frac{I_2^\pm}{I_6^\pm}\right]. \tag{A7}$$

Finally, by introducing the quantum Bohm potential Q_B, we report the following useful identities:

$$Q_B = -\frac{\hbar^2}{8m}\left\{2\frac{\partial^2 \ln n}{\partial x_r\,\partial x_r} + \left(\frac{\partial \ln n}{\partial x_r}\right)^2\right\}, \tag{A8}$$

$$n\frac{\partial Q_B}{\partial x_i} = -\frac{\hbar^2}{4m}\frac{\partial}{\partial x_k}\left\{n\frac{\partial^2 \ln n}{\partial x_i\,\partial x_k}\right\}, \tag{A9}$$

$$\frac{\partial n}{\partial x_i}Q_B = -\frac{\hbar^2}{8m}\frac{\partial}{\partial x_k}\left\{n\left[2\frac{\partial \ln n}{\partial x_i}\frac{\partial \ln n}{\partial x_k} - \left(\frac{\partial \ln n}{\partial x_r}\right)^2\delta_{ik}\right]\right\}. \tag{A10}$$

APPENDIX B

1. Fermi and Bose statistics of a weakly degenerate gas

For a weakly degenerate gas, the following series can be employed [31] when $\alpha > 1$:

$$I_n^\pm(\alpha) = \frac{1}{2}\Gamma\left(\frac{n+1}{2}\right)e^{(-\alpha)}\sum_{r=0}^{\infty}\frac{(\mp 1)^r}{(r+1)^{(n+1)/2}}e^{(-r\alpha)}. \tag{B1}$$

Completely nondegenerate case. We remark that, for $\alpha \gg 1$, we can use only the first term of this expansion, by recovering the results obtained in the framework of Boltzmann statistics, i.e., in the *completely nondegenerate* case. Thus, we have

$$I_n^\pm(\alpha_{ND}) \approx \frac{1}{2}\Gamma\left(\frac{n+1}{2}\right)\exp(-\alpha_{ND}), \tag{B2}$$

and using Eqs. (33), (A3), (A4), and (A8) we obtain

$$\exp(-\alpha_{ND}) \approx \frac{4\gamma}{\sqrt{\pi}}\frac{n}{T^{3/2}}\left[1 + \frac{Q_B}{3k_BT}\right] + \mathcal{O}(\hbar^4). \tag{B3}$$

Consequently, in the case of *completely nondegenerate Fermi and Bose gases* we obtain, up to terms of order $\hbar^2$, expression (36) for the quantum chemical potential $\mu = -\alpha_{ND}k_BT$. Analogously, if we insert functions (B2) in Eqs. (35), (49), (66)–(69), and (A3)–(A5), then we obtain, respectively, the quantum expressions (37) and (50) for the pressure and for the stress deviator, and the closure relations (70)–(73) for a completely nondegenerate gas.

Weakly degenerate case. By considering, for the integral functions $I_n^\pm(\alpha)$, the first two terms of expansion (B1) we include the effects of *weakly degenerate* case, being

$$I_n^\pm(\alpha) \approx \frac{1}{2}\Gamma\left(\frac{n+1}{2}\right)e^{(-\alpha)}\left[1 \mp \frac{e^{(-\alpha)}}{2^{(n+1)/2}}\right]. \tag{B4}$$

By inserting functions (B4) in Eq. (33), and by considering the right-hand side of this equation up to terms of order $\chi^{(0)} = (4\gamma/\sqrt{\pi})(n/T^{3/2}) \ll 1$, we obtain

$$\frac{1}{2}\Gamma\left(\frac{3}{2}\right)e^{(-\alpha)}\left[1 \mp \frac{e^{(-\alpha)}}{2^{3/2}}\right] \approx \gamma\frac{n}{T^{3/2}}\left[1 + \frac{Q_B}{3k_BT} \mp \frac{\chi^{(0)}}{2^{3/2}}\frac{(Q_B - Q_C)}{3k_BT}\right] + \mathcal{O}(\hbar^4), \tag{B5}$$

where Q_C is expressed by Eq. (40). Recalling that $\exp(-\alpha) \ll 1$, the second approximation for $\exp(-\alpha)$ is obtained by means of the relation

$$e^{(-\alpha)} \approx \chi^{(0)}\left\{1 + \frac{Q_B}{3k_BT} \mp \frac{\chi^{(0)}}{2^{3/2}}\frac{(Q_B - Q_C)}{3k_BT}\right\} \times \left[1 \mp \frac{1}{2^{3/2}}\exp(-\alpha_{ND})\right]^{-1}. \tag{B6}$$

By inserting Eq. (B3) in Eq. (B6), and considering only terms up to order $\hbar^2$ and up to order $(\chi^{(0)})^2$, we obtain

$$e^{(-\alpha)} \approx \chi^{(0)}\left\{\left(1 \pm \frac{\chi^{(0)}}{2^{3/2}}\right)\left[1 + \frac{Q_B}{3k_BT}\right] \pm \frac{\chi^{(0)}}{2^{3/2}}\frac{Q_C}{3k_BT}\right\} + \mathcal{O}(\hbar^4). \tag{B7}$$

Thus, being $\chi^{(0)} \ll 1$, we have as second approximation

$$-\alpha \approx \ln\left[\left(1 \pm \frac{\chi^{(0)}}{2^{3/2}}\right)\chi^{(0)}\right] + \frac{1}{3k_BT}\left(Q_B \pm \frac{\chi^{(0)}}{2^{3/2}}Q_C\right) + \mathcal{O}(\hbar^4).$$

In this way we determine the statistical quantum correction in Eq. (38) for the chemical potential μ. Analogously, if we use functions (B4) in Eqs. (35), (A3), and (A4) we have

$$P \approx nk_BT\left[1 \pm \frac{1}{2^{5/2}}\exp(-\alpha_{ND})\right] - \frac{\hbar^2}{36}\frac{n}{m}\left\{\left(1 \mp \frac{9}{2^{5/2}}\chi^{(0)}\right)\frac{\partial^2 \ln n}{\partial x_r\,\partial x_r} \mp \frac{17}{2^{7/2}}\chi^{(0)}\left(\frac{\partial \ln n}{\partial x_r}\right)^2\right\},$$

and by inserting Eq. (B3), we obtain the quantum second approximation in Eq. (39) for the pressure. Finally, we can use Eqs. (49), (A5), and (B4) to determine the second explicit approximation in Eq. (53) for the stress deviator.

2. Fermi statistics of a strongly degenerate gas

For the Fermi-Dirac statistics under strong degeneracy we can apply the asymptotic expansion due to Sommerfeld [31] for the functions $I_n^+(\alpha)$ (with $-\alpha \gg 1$).

Completely degenerate case. We start by considering a Fermi gas at absolute zero. In this case, when $T \to 0$, degeneracy becomes complete and it is possible to consider the approximation

$$I_n^+(\alpha_{CD}) \approx \frac{1}{n+1}(-\alpha_{CD})^{(n+1)/2}. \tag{B8}$$

Thus, by defining the quantity $\mu^{(0)}=(5\nu_F/2)n^{2/3}$ with $\nu_F=(\hbar^2/5m)[6\pi^2/(2\tilde{s}+1)]^{2/3}$, we insert the Fermi integrals of Eq. (B8) in Eqs. (33), (A3), and (A4) and by using identity (A8) we obtain the first approximation for α,

$$-\alpha_{CD} \approx \frac{\mu^{(0)}}{k_BT} + \frac{Q_B}{9k_BT} + \mathcal{O}(\hbar^4), \tag{B9}$$

and, consequently, Eq. (41) for the chemical potential. Analogously, with this procedure, we use Eqs. (B8), (B9), (35), (49), and (A3)–(A5) to determine the quantum approximations in Eqs. (42) and (56) for the pressure and for the stress deviator, in the case of a completely degenerate Fermi gas.

Strongly degenerate case. In the case of strongly degenerate Fermi gases, with $T > 0$, we can consider the first term of the asymptotic Sommerfeld expansion. Thus, for even values of n, we have the expressions

$$I_n^+(\alpha) \approx \frac{1}{n+1}(-\alpha)^{(n+1)/2}\left[1+\frac{\pi^2}{24}(n^2-1)\frac{1}{(-\alpha)^2}\right]. \tag{B10}$$

By inserting the Fermi integrals of Eq. (B10) in Eq. (33), and by considering the right-hand side of this equation up to terms of order $(k_BT/\mu^{(0)})^2 \ll 1$, we obtain

$$\frac{(-\alpha)^{3/2}}{3}\left[1+\frac{\pi^2}{8}\frac{1}{(-\alpha)^2}\right] = \gamma\frac{n}{T^{3/2}}\left\{1+\frac{1}{6\mu^{(0)}}\left[Q_B+\frac{\pi^2}{12}\left(\frac{k_BT}{\mu^{(0)}}\right)^2(\tilde{Q}_C-Q_B)\right]\right\} + \mathcal{O}(\hbar^4), \tag{B11}$$

where $\tilde{Q}_C$ is expressed by Eq. (45). Recalling that $-\alpha \gg 1$, the second approximation for $-\alpha$ is given by means of the relation

$$-\alpha \approx \frac{(3\gamma n)^{2/3}}{T}\left\{1+\frac{1}{6\mu^{(0)}}\left[Q_B+\frac{\pi^2}{12}\left(\frac{k_BT}{\mu^{(0)}}\right)^2(\tilde{Q}_C - Q_B)\right]\right\}^{2/3}\left[1+\frac{\pi^2}{8}\frac{1}{(-\alpha_{CD})^2}\right]^{-2/3}. \tag{B12}$$

Thus, by inserting Eq. (B9) in Eq. (B12), and considering only terms up to order $\hbar^2$ and up to order $(k_BT/\mu^{(0)})^2 \ll 1$, we obtain

$$-\alpha = \frac{\mu^{(0)}}{k_BT}\left[1-\frac{\pi^2}{12}\left(\frac{k_BT}{\mu^{(0)}}\right)^2\right] + \frac{1}{9k_BT}\left[Q_B+\frac{\pi^2}{12}\left(\frac{k_BT}{\mu^{(0)}}\right)^2\tilde{Q}_C\right] + \mathcal{O}(\hbar^4), \tag{B13}$$

and, consequently, the second quantum approximation in Eq. (43) for the chemical potential. Analogously, with this procedure, we can use Eqs. (B10), (B13), (35), (49), and (A3)–(A5) to determine the explicit second quantum approximations in Eqs. (44) and (59) for the pressure and for the stress deviator, in the case of a strongly degenerate Fermi gas.

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