# A PROPER NONLOCAL FORMULATION OF QUANTUM MAXIMUM ENTROPY PRINCIPLE FOR FERMI, BOSE AND FRACTIONAL ESCLUSION STATISTICS

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### ABSTRACT

By considering the Wigner formalism 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. From one hand, the main difficulty in QMEP is to define an appropriate quantum entropy that explicitly incorporates quantum statistics. From another hand, the availability of rigorous quantum hydrodynamic (QHD) models is a demanding issue for a variety of quantum systems like, interacting fermionic and bosonic gases, confined carrier transport in semiconductor heterostrucures, anyonic systems, etc. We present a rigorous nonlocal formulation of QMEP by defining a quantum entropy that includes Fermi, Bose and, more generally, fractional exclusion statistics. In particular, by considering anyonic systems satisfying fractional exclusion statistic, all the results available in the literature are generalized in terms of both the kind of statistics and a nonlocal description for excluson gases. Finally, gradient quantum corrections are explicitly given at different levels of degeneracy and classical results are recovered when  $\hbar$  tends to 0.

## INTRODUCTION

In thermodynamics and statistical mechanics entropy is the fundamental physical quantity to describe the evolution 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  $\Gamma$  is the number of microstates exploiting the given macroscopic properties. In this context, it is well known that in classical mechanics the entropy: i) allows the violation of the uncertainty principle [1]; ii) can be considered as a special case of the so-called *Boltzmann-Gibbs-Shannon* entropy that enables one to apply results of information theory to physics [1; 2]. In particular, maximum entropy principle (MEP) allows one to derive [2; 3; 4; 5] the nonequilibrium distribution function associated with particles, and to determine the microstate corresponding to the given macroscopic quantity.

We remak, that the MEP can be exploited in the completely nonlinear case, without any assumption on the nonequilibrium processes. Alternatively, an approximate distribution function is usually derived through a formal expansion around a local equilibrium configuration and so Extended Thermodynamics (ET) theories [3; 6] of  $\mathcal{N}$  moments and degree  $\alpha$  ( $ET^{\alpha}_{\mathcal{N}}$  models) were obtained. In this way, it was found possible to derive rigorous hydrodynamic (HD) models based on the *moments* of the distribution function to different orders of a power expansion and including appropriate closure conditions [3; 6; 7; 8]. Accordingly, making use of the Lagrange multipliers technique, it was found possible to construct the set of evolution equations for the macro-variables of interest.

Apart from some partial attempts [2; 9; 10], this is no longer the case in quantum mechanics. Here, the main difficulties concern with: i) the definition of a proper quantum entropy that includes particle indistinguishability; ii) the formulation of a global quantum MEP (QMEP) that allows one to obtain a quantum distribution function both for thermodynamic equilibrium and nonequilibrium configurations. From one hand, in the framework of a nonlocal quantum theory, the generalization of the corresponding Lagrange multipliers is also an open problem. From another hand, a 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, anyonic systems, quantum turbulence, quantum fluids, quantized vortices, nuclear physics, confined carrier transport in semiconductor heterostrucures, phonon and electron transport in nanostructures, nanowires and thin layers.

Recently, a comprehensive review on QMEP which summarizes the state-of-the-art on this subject was presented in Ref. [8]. Accordingly, all the results available from the literature for a three-dimensional (3D) Fermi and/or Bose gas, have been generalized in the framework of a nonlocal Wigner theory both in equilibrium and nonequilibrium conditions [11].

The aim of this work is to consider an extension of QMEP in the framework of fractional exclusion statistics (FES). In particular we consider anyonic systems satisfying FES [12], and to determine the thermodynamic evolution of an excluson gas compatibly with the uncertainty principle. In this way, within the framework of a QMEP-Wigner formulation, we generalize all the results available from the literature in terms of both: the kind of statistics and a nonlocal description for the quantum gas.

#### FRACTIONAL STATISTICS

Whereas fermions and bosons can exist in all dimensions, certain low dimensional systems have elementary excitations that may obey quantum statistics interpolating between fermionic and bosonic behaviors. In particular, particles carrying these generalized statistics, are called generically *anyons*  [13]. For anyons, fractional statistics are related to the trajectory dependence in the particle exchange procedure in configuration space and are connected to the braid group structure of particle trajectories [13; 14; 15] in two spatial dimensions (2D). Mathematically, fractional statistics are parameterized by a phase factor that describes how the field operators of an anyonic system changes because of exchange procedure in 2D configuration space [13; 14; 15]. Thus, the concept of anyons is specific to two dimensions, and because of the trajectory dependence, the single particle state is inextricably connected with the complete state of the many-body configuration of the system. In 2D systems, the fractional statistics have been successfully applied to describe the charged excitations (Laughlin quasi-particles [16]) of a fractional quantum Hall (FQH) [17] where the electron gas shows a fractional electric charge [18] and, more recently, a direct evidence of fractional exchange phase factor was observed in experiments [19]. We remark, that fractional anyon statistics has been formalized, to some extent [20; 21], also in the onedimensional (1D) case. In particular, for 1D systems the interactions and statistics are inextricably related, because the collision phenomena are the only way to interchange two particles. Accordingly, also in this case, anyons acquire a step-functionlike phase when two identical particles exchange their positions in the scattering process. Anyons in 1D models are still unexplored to a wide extent, although many one-dimensional anyonic models have been introduced and investigated in literature [22; 23; 24; 25; 26; 27] Thus, by defining the q-deformed bracket  $[A,B]_q = AB - qBA$ , we can introduce (for D = 1,2) the anyon field operators  $\Psi(\mathbf{r})$  and  $\Psi^{\dagger}(\mathbf{r})$  with the general deformed relations [14; 28; 29]

$$\left[ \Psi(\mathbf{r}), \Psi(\mathbf{r}') \right]_q = \left[ \Psi^{\dagger}(\mathbf{r}), \Psi^{\dagger}(\mathbf{r}') \right]_q = 0, \tag{1}$$

$$\left[\Psi(\mathbf{r}), \Psi^{\dagger}(\mathbf{r}')\right]_{q^{-1}} = \delta^{D}(\mathbf{r} - \mathbf{r}'), \qquad (2)$$

where  $q(\mathbf{r}, \mathbf{r'})$  is a discontinuous function of its arguments [14; 29] corresponding to a phase factor that denotes the system statistics [30] and, for the sake of consistency

$$q(\mathbf{r},\mathbf{r}') = q^{-1}(\mathbf{r}',\mathbf{r}), \text{ with } q(\mathbf{r},\mathbf{r}) = \pm 1,$$
 (3)

A different notion of fractional statistics, in arbitrary dimension D, has been introduced by Haldane [31]. This approach is based on a generalized Pauli exclusion principle where it is necessary to count as changes the dimension of the single particle Hilbert space when extra particles are added, keeping constant both the boundary conditions and the size of the condensed-matter region. Particles that obey Haldane exclusion-statistics (HES) are called exclusons with (in the case of single specie) a statistics parameter  $\kappa = -\delta G / \delta N$ , where  $\delta G$  describes the change in size of the subset of available single-particle states corresponding to a variation of  $\delta N$  particles. It is known that HES is, in general, different from anyon statistics. Indeed, the excluson statistics is assigned to elementary excitations of condensed matter systems, which are not necessarily connected with braiding considerations [21; 31]. However, there are some systems where a thermodynamics coincidence of the two statistics was shown [22; 25; 31; 32]. In this case, it is possible to think that the anyon model is a microscopic quantum realization of Haldane statistics.

In the next sections we consider anyonic systems satisfying the FES, to describe the thermodynamic evolution of an excluson gas by using QMEP-Wigner formalism. In this way, compatibly with the uncertainty principle, we include both the statistical effects and a nonlocal description for the system.

### THE WIGNER DYNAMICS

Following Ref. [8; 12] we consider a fixed number *N* of identical particles and introduce in Fock space the statistical density matrix  $\rho$  for the whole system, with  $Tr(\rho) = 1$ , (we suppress the symbol  $\hat{}$  to refer to operators acting in Fock space) and the general Hamiltonian [33]

$$H = \int d^3 r \Psi^{\dagger}(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \Psi(\mathbf{r}) +$$

$$\frac{1}{2} \int \int d^D r d^D r' \Psi^{\dagger}(\mathbf{r}) \Psi^{\dagger}(\mathbf{r}') V(\mathbf{r},\mathbf{r}') \Psi(\mathbf{r}') \Psi(\mathbf{r})$$
(4)

where *m* is the particle effective mass,  $U(\mathbf{r})$  is the one-body potential,  $V(\mathbf{r}, \mathbf{r}')$  is a two-body symmetric interaction potential,  $\Psi$  and  $\Psi^{\dagger}$  are wave field operators satisfying the anyon relations (1)-(3) with their properties [30; 33]. Analogously, in coordinate space representation, we define the reduced density matrix [8; 11] of single particle (here and henceforth we use the symbol  $\widehat{}$  for single particle operators)  $\langle \mathbf{r} | \widehat{\rho} | \mathbf{r}' \rangle = \langle \Psi^{\dagger}(\mathbf{r}') \Psi(\mathbf{r}) \rangle = Tr(\rho \Psi^{\dagger}(\mathbf{r}') \Psi(\mathbf{r}))$  that in an arbitrary representation takes the form  $\langle \mathbf{v} | \widehat{\rho} | \mathbf{v}' \rangle = \langle a_{v'}^{\dagger} a_{v} \rangle = Tr(\rho a_{v'}^{\dagger} a_{v})$  being  $\mathbf{v}, \mathbf{v}'$  single particle states,  $a_{v}, a_{v'}^{\dagger}$  annihilation and creation operators for these states and  $\langle \cdots \rangle$  the statistical mean value. Thus, if we consider a one-particle observable  $\widehat{\mathcal{M}}$  then an ensemble average will lead to the expected value  $Tr(\widehat{\rho} \widehat{\mathcal{M}}) = \int d^D r d^D r' \langle \Psi^{\dagger}(\mathbf{r}') \Psi(\mathbf{r}) \rangle \langle \mathbf{r}' | \widehat{\mathcal{M}} | \mathbf{r} \rangle$ . By using this formalism, we can define the *reduced* Wigner function

$$\mathcal{F}_{\mathcal{W}} = \frac{1}{(2\pi\hbar)^D} \int d^D \tau e^{-\frac{i}{\hbar} \tau \cdot \mathbf{p}} \langle \Psi^{\dagger}(\mathbf{r} - \tau/2) \Psi(\mathbf{r} + \tau/2) \rangle \quad (5)$$

with  $\int d^D p \mathcal{F}_{\mathcal{W}} = \langle \mathbf{r} | \hat{\boldsymbol{\rho}} | \mathbf{r} \rangle = \langle \Psi^{\dagger}(\mathbf{r}) \Psi(\mathbf{r}) \rangle = n(\mathbf{r})$ , being  $n(\mathbf{r})$  the quasi-particle numerical density, with  $Tr(\hat{\boldsymbol{\rho}}) = N$ .

Accordingly, by considering an operator of single particle  $\widehat{\mathcal{M}}(\widehat{\mathbf{r}}, \widehat{\mathbf{p}})$ , we look for a function  $\widetilde{\mathcal{M}}(\mathbf{r}, \mathbf{p})$  in phase space that *corresponds* unambiguously to operator  $\widehat{\mathcal{M}}$ , introducing the Weyl-Wigner transform  $\mathcal{W}(\widehat{\mathcal{M}}) = \widetilde{\mathcal{M}}(\mathbf{r}, \mathbf{p}) = \int d^D \tau \langle \mathbf{r} + \tau/2 | \widehat{\mathcal{M}} | \mathbf{r} - \tau/2 \rangle e^{-\frac{i}{\hbar} \tau \cdot \mathbf{p}}$  and, analogously, we define the inverse Wigner transform  $\mathcal{W}^{-1}(\widetilde{\mathcal{M}}) = \langle \mathbf{r} | \widehat{\mathcal{M}} | \mathbf{r}' \rangle = (2\pi\hbar)^{-D} \int d^D p \, \widetilde{\mathcal{M}}((\mathbf{r} + \mathbf{r}')/2, \mathbf{p}) e^{\frac{i}{\hbar} \mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')}$  which maps the function  $\widetilde{\mathcal{M}}$  on phase space into the operator  $\widehat{\mathcal{M}}$ .

Thus, by using the equation of motion in the Heisenberg picture  $i\hbar\partial_t\Psi(\mathbf{r}) = [\Psi(\mathbf{r}), H]$ , the relations (1)-(3) with their properties[30], and the symmetry of terms  $V(\mathbf{r}, \mathbf{r}')$ , we obtain the equations  $i\hbar\partial_t\Psi(\mathbf{r}) = \mathcal{H}(\mathbf{r})\Psi(\mathbf{r})$  and  $-i\hbar\partial_t\Psi^{\dagger}(\mathbf{r}) = \Psi^{\dagger}(\mathbf{r})\mathcal{H}(\mathbf{r})$  with

$$\mathcal{H}(\mathbf{r}) = -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) + \int d^D r' \Psi^{\dagger}(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \Psi(\mathbf{r}'). \quad (6)$$

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 obtain, in the generalized Hartree approximation [34], the usual evolution-equation for the reduced density matrix of single particle

$$i\hbar\frac{\partial}{\partial t}\langle \mathbf{r}|\widehat{\boldsymbol{\rho}}|\mathbf{r}'\rangle = \int d^{D}r''[\langle \mathbf{r}|\widehat{\mathcal{H}}|\mathbf{r}''\rangle\langle \mathbf{r}''|\widehat{\boldsymbol{\rho}}|\mathbf{r}'\rangle - \langle \mathbf{r}|\widehat{\boldsymbol{\rho}}|\mathbf{r}''\rangle\langle \mathbf{r}''|\widehat{\mathcal{H}}|\mathbf{r}'\rangle] \quad (7)$$

being  $\widehat{\mathcal{H}} = \langle \mathcal{H} \rangle$  the single particle Hamilton operator. Accordingly, following a usual script [8; 11; 34], we can use all previous relations to obtain the formal full expansion, to all orders in  $\hbar$ , of the Wigner equation in the generalized Hartree approximation

$$\frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial t} + \frac{p_k}{m} \frac{\partial \mathcal{F}_{\mathcal{W}}}{\partial x_k} =$$

$$\sum_{l=0}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \left[ \frac{\partial^{2l+1} V_{eff}}{\partial x_{k_1} \cdots \partial x_{k_{2l+1}}} \right] \left[ \frac{\partial^{2l+1} \mathcal{F}_{\mathcal{W}}}{\partial p_{k_1} \cdots \partial p_{k_{2l+1}}} \right]$$
(8)

where all effects of the interactions are entirely contained in the definition of the effective potential [35],  $V_{eff}(\mathbf{r}) = U(\mathbf{r}) + \int d^D r' n(\mathbf{r}') V(\mathbf{r}, \mathbf{r}')$ .

## QUANTUM ENTROPY AND QMEP FORMALISM

The most used definition of quantum entropy is due to Von Neumann [36], and is expressed in the form

$$S = -k_B T r(\rho \ln \rho) \tag{9}$$

where  $\rho$  is the statistical density matrix operator appropriate to the physical system under study.

Although the relation (9) 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 stems in the fact that it does not include the statistical effects for a system of identical particles. To account for the effects of statistics in Eq. (9), it is mandatory to consider an additional information specifying whether the density operator  $\rho$ , defined in Fock space, is associated with an excluson system, fermion or boson like. In order to take into account *ab initio* the statistics for a system of identical particles, we can follow the usual strategy of evaluating the quantum entropy as the logarithm of the *statistical weight* for the whole system.

Thus, to take into account *ab initio* the FES, we evaluate the entropy *S* for a noninteracting system under nonequilibrium conditions in terms of the occupation numbers [37]

$$S = -k_B \sum_{\mathbf{v}} y \left\{ \langle \overline{N_{\mathbf{v}}} \rangle \ln \langle \overline{N_{\mathbf{v}}} \rangle + (1 - \kappa \langle \overline{N_{\mathbf{v}}} \rangle) \ln (1 - \kappa \langle \overline{N_{\mathbf{v}}} \rangle) - [1 + (1 - \kappa) \langle \overline{N_{\mathbf{v}}} \rangle] \ln [1 + (1 - \kappa) \langle \overline{N_{\mathbf{v}}} \rangle] \right\}$$
(10)

with  $\langle \overline{N_v} \rangle = \langle a_v^{\dagger} a_v \rangle / y$ , y the spin degeneration, and  $\kappa$  the statistical parameter of fractional statistics. If we consider the Schrödinger equation of single particle  $[\widehat{\mathcal{H}}(\mathbf{r}) - E_v] \varphi_v(\mathbf{r}) = 0$  then, the occupation numbers  $\langle N_v \rangle$ , associated with the energies  $E_v$ , will completely specify the macroscopic state of the gas. In particular, by using the relation (7) in stationary conditions, both the *reduced density matrix* and any operator  $\widehat{\Phi}(\widehat{\rho})$  are diagonal in the base  $\varphi_v$ . Therefore, by introducing as function of  $\widehat{\rho}$  the quantity

$$\widehat{\Phi}(\widehat{\rho}) = y \left\{ \frac{\widehat{\rho}}{y} \ln\left(\frac{\widehat{\rho}}{y}\right) + \left(\widehat{I} - \kappa\frac{\widehat{\rho}}{y}\right) \ln\left(\widehat{I} - \kappa\frac{\widehat{\rho}}{y}\right) - \left[\widehat{I} + (1 - \kappa)\frac{\widehat{\rho}}{y}\right] \ln\left[\widehat{I} + (1 - \kappa)\frac{\widehat{\rho}}{y}\right] \right\}$$
(11)

with  $\widehat{I}$  the identity, we obtain  $\langle v | \widehat{\rho} | v' \rangle = \langle a_v^{\dagger} a_v \rangle \delta_{vv'}$  and

$$\begin{aligned} \langle \mathbf{v} | \widehat{\Phi}(\widehat{\rho}) | \mathbf{v}' \rangle &= y \left\{ \langle \overline{N_{\mathbf{v}}} \rangle \ln \langle \overline{N_{\mathbf{v}}} \rangle + (1 - \kappa \langle \overline{N_{\mathbf{v}}} \rangle) \ln (1 - \kappa \langle \overline{N_{\mathbf{v}}} \rangle) - \\ & \left[ 1 + (1 - \kappa) \langle \overline{N_{\mathbf{v}}} \rangle \right] \ln \left[ 1 + (1 - \kappa) \langle \overline{N_{\mathbf{v}}} \rangle \right] \right\} \delta_{\mathbf{v}\mathbf{v}'} \end{aligned}$$
(12)

We remark, that for  $\kappa = 1$  or  $\kappa = 0$  the entropy (10) recovers the usual expressions for fermions or bosons [38], and Eqs. (11)-(12) become

$$\begin{split} \widehat{\Phi}(\widehat{\rho}) &= \widehat{\rho} \left\{ \ln\left(\frac{\widehat{\rho}}{y}\right) \pm y \widehat{\rho}^{-1} \left(\widehat{I} \mp \frac{\widehat{\rho}}{y}\right) \ln\left(\widehat{I} \mp \frac{\widehat{\rho}}{y}\right) \right\} (13) \\ \langle \nu | \widehat{\Phi}(\widehat{\rho}) | \nu' \rangle &= y \left[ \langle \overline{N_{\nu}} \rangle \ln \langle \overline{N_{\nu}} \rangle \pm \left(1 \mp \langle \overline{N_{\nu}} \rangle \right) \times (14) \\ \ln \left(1 \mp \langle \overline{N_{\nu}} \rangle \right) \right] \delta_{\nu\nu'} \end{split}$$

Analogously, under nondegenerate conditions Bose and Fermi statistics tend to Boltzmann statistics as limit case, and the general expressions (11)-(12) reduce to

$$\widehat{\Phi}(\widehat{\rho}) = \widehat{\rho} \left\{ \ln\left(\frac{\widehat{\rho}}{y}\right) - \widehat{I} \right\},\tag{15}$$

$$\langle \nu | \widehat{\Phi}(\widehat{\rho}) | \nu' \rangle = y \langle \overline{N_{\nu}} \rangle \left( \ln \langle \overline{N_{\nu}} \rangle - 1 \right) \delta_{\nu \nu'}. \tag{16}$$

Consequently, by generalizing existing definitions [1; 2; 9; 10; 36], the statistics can be implicitly taken into account by defining, for the whole system, the quantum entropy in terms of the functional of the reduced density matrix

$$S(\widehat{\rho}) = -k_B T r[\widehat{\Phi}(\widehat{\rho})] \tag{17}$$

where  $\widehat{\Phi}(\widehat{\rho})$  is given by Eq. (11) for the FES [12], by Eq. (13) for the Fermi or Bose gases [8; 11], and by Eq. (15) for the Boltzmann gas.

#### General formulation of QMEP in phase space

By considering an arbitrary set of single-particle observable  $\{\widehat{\mathcal{M}}_A\}$  and the corresponding space-phase functions  $\{\widetilde{\mathcal{M}}_A\}$ , we define the macroscopic *local moments* 

$$M_A(\mathbf{r},t) = \int d^D p \ \widetilde{\mathcal{M}}_A(\mathbf{r},\mathbf{p}) \ \mathcal{F}_{\mathcal{W}}(\mathbf{r},\mathbf{p},t)$$
(18)

and we use the functional (17) as an *informational entropy* for the system. To formulate the QMEP in phase space, we introduce the phase function  $\tilde{\Phi}(\mathbf{r},\mathbf{p}) = \mathcal{W}(\hat{\Phi}(\hat{\rho}))$ , we rewrite Eq. (17) in the form

$$S(\widehat{\rho}) = -\frac{k_B}{(2\pi\hbar)^D} \int \int d^D p \, d^D r \, \mathcal{W}(\widehat{\Phi}(\widehat{\rho})) \,, \qquad (19)$$

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  $\{M_A(\mathbf{r},t)\}$  with  $A = 1, \dots \mathcal{N}$ . To this purpose, we define the new *global* functional [8; 10; 11]

$$\widetilde{S} = S - \int d^D r \left\{ \sum_{A=1}^{\mathcal{N}} \widetilde{\lambda}_A \left[ \int d^D p \, \widetilde{\mathcal{M}}_A \, \mathcal{F}_{\mathcal{W}} - M_A \right] \right\}$$
(20)

being  $\tilde{\lambda}_A(\mathbf{r},t)$  the nonlocal *Lagrange multipliers* to be determined.

By using the general relation (11) introduced for the FES, one can show that the solution of the constraint  $\delta \tilde{S} = 0$  implies

$$\widehat{\rho} = y \left\{ \widehat{w}(\widehat{\xi}) + \kappa \widehat{I} \right\}^{-1}$$
(21)

where the operator  $\hat{w}$  satisfies the functional relation

$$[\widehat{w}(\widehat{\xi})]^{\kappa}[\widehat{I} + \widehat{w}(\widehat{\xi})]^{1-\kappa} = \widehat{\xi}$$
(22)

with the operator

$$\widehat{\xi} = \exp\left[\mathcal{W}^{-1}\left(\sum_{A=1}^{\mathcal{N}} \lambda_A \,\widetilde{\mathcal{M}}_A\right)\right] \quad \text{and} \quad \lambda_A = \frac{\widetilde{\lambda}_A}{k_B} \tag{23}$$

The set of Eqs. (21)-(23) is a first major result. It generalizes existing results [37], in an operatorial sense, under both thermodynamic equilibrium and nonequilibrium conditions. Besides, the relations (21)-(23), together with Eqs. (11) and (17), provide a generalized definition of quantum entropy that includes nonlocal effects in FES. As a consequence, a nonlocal Wignertheory for the system can be formulated by explicitly evaluating the corresponding reduced Wigner-function

$$\mathcal{F}_{\mathcal{W}} = (2\pi\hbar)^{-D} \, \mathcal{W}(\widehat{\rho}[\lambda_A(\mathbf{r},t),\mathcal{M}_A]). \tag{24}$$

We note, that by solving the general relation (22) for  $\kappa = 1,0$  we reobtain the Fermi and Bose statistics, being in this case [8; 11]

$$\widehat{\boldsymbol{\rho}} = y \left\{ \exp\left[ \mathcal{W}^{-1} \left( \sum_{A=1}^{\mathcal{N}} \lambda_A(\mathbf{r}, t) \, \widetilde{\mathcal{M}}_A \right) \right] \pm \widehat{I} \right\}^{-1}$$
(25)

while for the Boltzmann statistics, we obtain the simplified expression

$$\widehat{\boldsymbol{\rho}} = y \exp\left\{ \mathcal{W}^{-1} \left( -\sum_{A=1}^{\mathcal{N}} \lambda_A(\mathbf{r}, t) \, \widetilde{\mathcal{M}}_A \right) \right\}$$
(26)

We conclude by remarking that, 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 include the microscopic kinetic details, (ii) to determine the Lagrange multipliers in terms of these constraints. In this way, the QMEP approach implicitly includes all the kinetic details of the microscopic interactions among particles. Then, by knowing the functional form (21)-(24) of the reduced Wigner function, we use Eq. (8) to obtain a set of evolution equations for the constraints. This set completely represents the QHD model in which all the constitutive functions are determined starting from their kinetic expressions. 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 obtain order by order corrections terms.

### Moyal expansion of the Wigner function

By using the Moyal formalism [39], one can prove that the phase function  $\widetilde{w} = \mathcal{W}(\widehat{w})$ , the Wigner function  $\mathcal{F}_{\mathcal{W}}$  and, hence, the moments  $M_A$  can be expanded in even power of  $\hbar$  as

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

To this end, the Lagrange multipliers  $\lambda_A$  must be determined by inverting, order by order, the constrains

$$M_A = \frac{1}{(2\pi\hbar)^D} \int d^D p \ \widetilde{\mathcal{M}}_A \ \mathcal{W}\left(\widehat{\rho}[\lambda_B(\mathbf{r},t),\widetilde{\mathcal{M}}_B]\right).$$
(27)

where the inversion problem can be solved [8; 11] only by assuming that also the Lagrange multipliers admit for an expansion in even powers of  $\hbar$ 

$$\lambda_A = \lambda_A^{(0)} + \sum_{k=1}^{\infty} \hbar^{2k} \lambda_A^{(2k)}, \qquad (28)$$

In this way, by using Eqs. (21)-(24) and (27)-(28), with the strategy reported in Ref. [8; 11], we succeed in determining the following expression for the reduced Wigner-function

$$\mathcal{F}_{W} = \frac{\widetilde{y}}{w^{(0)}(\xi) + \kappa} \left\{ 1 + \sum_{r=1}^{\infty} \hbar^{2r} \mathcal{P}_{2r} \right\},$$
(29)

where  $\tilde{y} = y/(2\pi\hbar)^D$ ,  $\xi = \exp(\Pi)$  with  $\Pi = \sum \lambda_A \widetilde{\mathcal{M}}_A$ , the nonlocal terms  $\mathcal{P}_{2r}$  expressed by recursive formulas and the function  $w^{(0)}$  satisfying the usual functional equation

$$[w^{(0)}(\xi)]^{\kappa}[1+w^{(0)}(\xi)]^{1-\kappa} = \xi.$$
(30)

Equation (29) is a second major result. Indeed, making use of  $\xi_0 = e^{\Pi_0}$  with  $\Pi_0 = \sum \lambda_A^{(0)} \widetilde{\mathcal{M}}_A$ , from (29) we obtain, explicitly, the following first order (r = 1) quantum correction

$$\mathcal{P}_{2} = \left\{ \frac{2}{[w^{(0)}(\xi_{0}) + \kappa]^{2}} \left( \xi_{0} \frac{dw^{(0)}}{d\xi_{0}} \right)^{2} - \frac{1}{w^{(0)}(\xi_{0}) + \kappa} \right. \\ \times \left[ \xi_{0}^{2} \frac{d^{2}w^{(0)}}{d\xi_{0}^{2}} + \xi_{0} \frac{dw^{(0)}}{d\xi_{0}} \right] \right\} \mathcal{H}_{2}^{(2)} - \left\{ \frac{6}{[w^{(0)}(\xi_{0}) + \kappa]^{2}} \right. \\ \left. \times \left[ \frac{1}{w^{(0)}(\xi_{0}) + \kappa} \left( \xi_{0} \frac{dw^{(0)}}{d\xi_{0}} \right)^{3} - \left( \xi_{0} \frac{dw^{(0)}}{d\xi_{0}} \right)^{2} - \right. \\ \left. \xi_{0}^{3} \frac{d^{2}w^{(0)}}{d\xi_{0}^{2}} \frac{dw^{(0)}}{d\xi_{0}} \right] + \frac{1}{w^{(0)}(\xi_{0}) + \kappa} \left[ \xi_{0}^{3} \frac{d^{3}w^{(0)}}{d\xi_{0}^{3}} + \right. \\ \left. 3\xi_{0}^{2} \frac{d^{2}w^{(0)}}{d\xi_{0}^{2}} + \xi_{0} \frac{dw^{(0)}}{d\xi_{0}} \right] \right\} \mathcal{H}_{3}^{(2)}$$

$$(31)$$

being the nonlocal functions  $\mathcal{H}_2^{(2)}$  and  $\mathcal{H}_3^{(2)}$  expressed by

$$\mathcal{H}_{3}^{(2)} = -\frac{1}{24} \left[ \frac{\partial^{2} \Pi_{0}}{\partial x_{i} \partial x_{j}} \frac{\partial \Pi_{0}}{\partial p_{i}} \frac{\partial \Pi_{0}}{\partial p_{j}} + \frac{\partial^{2} \Pi_{0}}{\partial p_{i} \partial p_{j}} \frac{\partial \Pi_{0}}{\partial x_{i}} \frac{\partial \Pi_{0}}{\partial x_{j}} \right]$$

$$-2\frac{\partial^2 \Pi_0}{\partial x_i \partial p_j}\frac{\partial \Pi_0}{\partial x_j}\frac{\partial \Pi_0}{\partial p_i}\bigg],\qquad(32)$$

$$\mathcal{H}_{2}^{(2)} = -\frac{1}{8} \left[ \frac{\partial^{2} \Pi_{0}}{\partial x_{i} \partial x_{j}} \frac{\partial^{2} \Pi_{0}}{\partial p_{i} \partial p_{j}} - \frac{\partial^{2} \Pi_{0}}{\partial x_{i} \partial p_{j}} \frac{\partial^{2} \Pi_{0}}{\partial x_{j} \partial p_{i}} \right].$$
(33)

#### We remark the following main points:

(i) For  $\kappa = 1$  and  $\kappa = 0$  we recover the gradient nonlocal results obtained for Fermi and Bose gases [8; 11], being in this case

$$\mathcal{F}_{\mathcal{W}} = \frac{\widetilde{y}}{e^{\Pi} \pm 1} \left\{ 1 + \sum_{r=1}^{\infty} \hbar^{2r} \mathcal{P}_{2r}^{\pm} \right\},$$
(34)

with the first quantum correction (31) that becomes

$$\mathcal{P}_{2}^{\pm} = \left\{ 6 \left[ \frac{e^{\Pi_{0}}}{e^{\Pi_{0}} \pm 1} \right]^{2} - 6 \left[ \frac{e^{\Pi_{0}}}{e^{\Pi_{0}} \pm 1} \right]^{3} - \frac{e^{\Pi_{0}}}{e^{\Pi_{0}} \pm 1} \right\} \mathcal{H}_{3}^{(2)} + \left\{ 2 \left[ \frac{e^{\Pi_{0}}}{e^{\Pi_{0}} \pm 1} \right]^{2} - \frac{e^{\Pi_{0}}}{e^{\Pi_{0}} \pm 1} \right\} \mathcal{H}_{2}^{(2)}$$
(35)

Analogously, by considering a quantum Boltzmann gas [8; 11], we obtain the simplified relations

$$\mathcal{F}_{\mathcal{W}} = \widetilde{y}e^{-\Pi} \left\{ 1 + \sum_{r=1}^{\infty} \hbar^{2r}\mathcal{P}_{2r} \right\} \quad \text{with} \quad \mathcal{P}_{2} = \mathcal{H}_{2}^{(2)} - \mathcal{H}_{3}^{(2)}$$
(36)

(ii) The functions  $\{\mathcal{H}_2^{(2)}, \mathcal{H}_3^{(2)}\}$  are in general, expressed in terms of the quantities  $\{M_A, \frac{\partial M_A}{\partial x_k}, \frac{\partial^2 M_A}{\partial x_i \partial x_k}, \mathbf{p}\}$ ; in any case, these functions can be evaluated using different levels of approximation [40].

(iii) In thermodynamics equilibrium conditions we can write  $\Pi|_E = \alpha + \beta \tilde{\epsilon}$  where  $\tilde{\epsilon} = m\tilde{u}^2/2$ , being  $\tilde{u}_i = u_i - \lambda_i$  the peculiar velocity,  $u_i = p_i/m$  the group velocity, and  $\{\alpha, \beta, \lambda_i\}$  the equilibrium nonlocal Lagrange multipliers.

#### EXAMPLES AND APPLICATIONS

As relevant application of the above results, we consider an excluson gas in isothermal equilibrium conditions. Accordingly,  $\beta = (k_B T)^{-1}$ , with *T* the constant temperature, and within a general approach all nonlocal effects can be described in terms of spatial derivatives of concentration  $n(\mathbf{r}, t)$  and mean velocity  $v_i(\mathbf{r}, t) = n^{-1} \int d^D p \, u_i \mathcal{F}_{\mathcal{W}}$ . In this case it is necessary to determine a closed set of balance equations for the variables  $\{n, v_i\}$  used as constraints in the QMEP procedure. Thus, by considering the kinetic fields  $\widetilde{\mathcal{M}}_A = \{1, u_i\}$  and using Eq. (8) we obtain the quantum drift-diffusion model [8; 11]

$$\dot{n} + n \frac{\partial v_k}{\partial x_k} = 0, \quad \dot{v}_i + \frac{1}{n} \frac{\partial M_{ik}}{\partial x_k} + \frac{1}{m} \frac{\partial V_{eff}}{\partial x_i} = 0, \quad (37)$$

where the unknown function  $M_{ik}$  can be decomposed as

$$M_{ik} = M_{\langle ik \rangle} + \frac{P}{m} \delta_{ik} + O(\hbar^4)$$
(38)

being the traceless part of tensor

$$M_{\langle ik 
angle} + O(\hbar^4) = \int d^D p \,\, ilde{u}_{\langle i} ilde{u}_{k 
angle} \,\, \mathcal{F}_{\mathcal{W}}$$

and the generalized quantum pressure

$$P + \mathcal{O}(\hbar^4) = rac{2}{D} \int d^D p \; \widetilde{\mathbf{\epsilon}} \; \mathcal{F}_{\mathcal{W}}|_E$$

independent constitutive quantities. Then, by making use of Eqs. (29)-(33), we calculate the variables of local equilibrium  $\{n, P\}$  and the traceless tensor  $M_{\langle ik \rangle}$ , determining the general relations

$$I_{D-1}(\alpha, \kappa) = \gamma \frac{n}{T^{D/2}} \left\{ 1 - \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[ \sum_{p=1}^2 \eta_{1p}^{(0)} Q^{(1,p)} + \eta_{21}^{(0)} Q^{(2,1)} \right] \right\} + O(\hbar^4)$$
(39)

$$P = \frac{2}{D} n k_B T \frac{I_{D+1}}{I_{D-1}} \left\{ 1 + \frac{\hbar^2}{12m} \frac{1}{k_B T} \left[ \sum_{p=1}^{2} \left( \eta_{1p}^{(1)} - \eta_{1p}^{(0)} \right) \times Q^{(1,p)} + \left( \eta_{21}^{(1)} - \eta_{21}^{(0)} \right) Q^{(2,1)} \right] \right\} + \mathcal{O}(\hbar^4)$$
(40)

$$M_{\langle ik \rangle} = -\frac{\hbar^2}{12} \frac{n}{m^2} (D-2) \frac{I_{D-3}}{I_{D-1}} Q_{\langle ik \rangle} + O(\hbar^4)$$
(41)

where  $\gamma = [\Gamma(D/2)/2y] (2\pi\hbar^2/mk_B)^{D/2}$ , the integral functions  $I_n(\alpha,\kappa)$ , the quantities  $\eta_{ij}^{(s)}$  and the nonlocal functions  $\{Q^{(q,p)}, Q_{\langle ik \rangle}\}$  are explicitly given in Eqs. (55) and (57)-(61) of Appendix.

By providing generalized differential constraints for the quantum system under interest, the relations (39)-(41) constitute a third major result. In particular, by solving Eq. (39) with respect to  $\alpha$ , we determine the generalized quantum chemical potential  $\mu = -\alpha k_B T$  and, by using Eq. (40), we obtain the generalized quantum equation of state. Thus, by introducing the usual Bohm quantum potential  $Q_B = -(\hbar^2/2m\sqrt{n}) \Delta \sqrt{n}$ , and the vorticity tensor  $T_{ij} = (\partial v_i/\partial x_j - \partial v_j/\partial x_i)$  the following simplified analytical cases are analyzed under isothermal equilibrium condition.

I) High-temperature and/or low-density limits.

*First approximation*: By using the first term of a suitable series expansion [41] for the functions  $I_n(\alpha, \kappa)$ , we obtain the completely nondegenerate case which is independent from  $\kappa$  (Boltzmann limit), being  $I_n^{\pm}(\alpha) \approx (1/2)\Gamma[(n+1)/2]\exp(-\alpha)$ . Thus, by defining the quantity  $\chi^{(0)} = y^{-1}[(2\pi\hbar^2)/(mk_B)]^{D/2}(n/T^{D/2})$  and using Eqs. (39)-(41) we obtain the generalized quantum expressions

$$\mu = k_B T \ln \left[ \chi^{(0)} \right] + \frac{Q'_B}{3} + O(\hbar^4), \qquad (42)$$

$$P = nk_BT + nQ_C^I + O(\hbar^4), \qquad (43)$$

with the first quantum nonlocal gradient corrections

$$Q_B^I = Q_B - \frac{\hbar^2}{16} \frac{\mathcal{T}_{ll}^2}{k_B T}$$

$$Q_C^I = -\frac{\hbar^2}{12D} \frac{1}{m} \left[ \frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \frac{m}{k_B T} T_{ll}^2 \right]$$

and the first approximation  $M^{I}_{\langle ik \rangle}$  for the tensor  $M_{\langle ik \rangle}$ 

$$M^{I}_{\langle ik\rangle} = -\frac{\hbar^{2}}{12} \frac{n}{m^{2}} \left[ \frac{\partial^{2} \ln n}{\partial x_{\langle i} \partial x_{k\rangle}} + \frac{m}{k_{B}T} \mathcal{T}^{2}_{\langle ik\rangle} \right] + O(\hbar^{4}).$$
(44)

By neglecting vorticity effects ( $T_{ik} = 0$ ) we recover relations well-known in literature [8; 11; 42], while, by including vorticity terms, we re-obtain some recent results for a quantum Boltzmann gas [43; 44].

Second approximation: By using the first two terms of the series expansion [41] we obtain  $I_n^{\pm}(\alpha, \kappa) \approx (1/2)\Gamma[(n+1)/2]\exp(-\alpha)\{1-(2\kappa-1)/2^{(n+1)/2}\exp(-\alpha)\}$ , and by considering Eqs. (39)-(41) and (57)-(61) with a standard iterative procedure [8; 11], we determine the correct quantum-statistical second approximation in terms of the quantity  $\chi^{(0)} \ll 1$ , being

$$\mu = k_B T \ln \left[ \left( 1 + \frac{2\kappa - 1}{2^{D/2}} \chi^{(0)} \right) \chi^{(0)} \right] + \frac{1}{3} \left( Q_B^I + \frac{2\kappa - 1}{2^{D/2}} \chi^{(0)} Q_B^{II} \right) + \mathcal{O}(\hbar^4)$$
(45)

$$P = nk_B T \left( 1 + \frac{2\kappa - 1}{2^{D/2 + 1}} \chi^{(0)} \right) + n \left( Q_C^I + \frac{2\kappa - 1}{2^{D/2 + 1}} \chi^{(0)} Q_C^{II} \right) + O(\hbar^4)$$
(46)

$$M_{\langle ik\rangle} = M^{I}_{\langle ik\rangle} + \frac{2\kappa - 1}{2^{D/2}} \chi^{(0)} M^{II}_{\langle ik\rangle} + \mathcal{O}(\hbar^4)$$
(47)

with the quantum nonlocal-gradient second corrections  $Q_B^{II}$ ,  $Q_C^{II}$  and  $M_{\langle ik \rangle}^{II}$  explicitly given in Eqs. (62)-(64) of Appendix.

II) low-temperature limits.

Under strong degeneracy, we make use of an asymptotic expansion [41] for the functions  $I_n(\alpha, \kappa)$  (with  $\kappa \in (0, 1]$ ).

First approximation: When  $T \to 0$  the degeneracy becomes complete and  $I_n(\alpha, \kappa) \approx (-\alpha)^{(n+1)/2} / [\kappa(n+1)]$ . Thus, by defining  $v_E = [4\pi/(D+2)](\hbar^2/m)[(\kappa/y)\Gamma(D/2+1)]^{2/D}$  and  $\mu^{(0)} = [(D+2)/2]v_E n^{2/D}$ , for  $\mu$  and P we obtain

$$\mu = \mu^{(0)} + \frac{D-2}{3D} Q_D^I + O(\hbar^4), \qquad (48)$$

$$P = v_E n^{(D+2)/D} + n Q_E^I + O(\hbar^4), \qquad (49)$$

with the quantum nonlocal-gradient first corrections

$$Q_D^I = Q_B - \frac{\hbar^2}{32} \frac{D}{\mu^{(0)}} \mathcal{T}_{ll}^2$$
$$Q_E^I = \frac{\hbar^2}{12D} \frac{1}{m} \left[ \frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \frac{2(D-1)}{D} \left( \frac{\partial \ln n}{\partial x_r} \right)^2 - \frac{m}{4} \frac{D}{\mu^{(0)}} \mathcal{T}_{ll}^2 \right]$$

and the first approximation  $\mathcal{M}^{I}_{\langle ik \rangle}$  for the tensor  $M_{\langle ik \rangle}$ 

$$\mathcal{M}_{\langle ik\rangle}^{I} = -\frac{\hbar^{2}}{12} \frac{n}{m^{2}} \left[ \frac{\partial^{2} \ln n}{\partial x_{\langle i} \partial x_{k\rangle}} + \frac{2}{D} \frac{\partial \ln n}{\partial x_{\langle i}} \frac{\partial \ln n}{\partial x_{k\rangle}} \right. \\ \left. + \frac{m}{2} \frac{D}{\mu^{(0)}} \mathcal{T}_{\langle ik\rangle}^{2} \right] + \mathcal{O}(\hbar^{4}).$$
(50)

In particular, for  $\kappa = 1$  (completely degenerate Fermi gas) and neglecting vorticity effects ( $\mathcal{T}_{ik} = 0$ ), we recover the gradient corrections obtained in the contest of Thomas-Fermi-Weizsacker theory [8; 11; 46]. For  $\kappa \neq 1$  and, by including also the vorticity terms, we generalize these results to excluson gases, in the low-temperature limit [12].

Second approximation: We consider the first two terms of the asymptotic expansion in series [41],  $I_n(\alpha, \kappa) \approx (-\alpha)^{(n+1)/2}/[\kappa(n+1)]\{1 + (\pi^2/24)\kappa(n^2 - 1)(-\alpha)^{-2}\}$ . Thus, by using Eqs. (39)-(41) and (57)-(61) with a suitable iterative procedure [8; 11], we obtain the second quantum-statistical correct approximation in terms of the quantities  $(k_B T/\mu^{(0)})^2 \ll 1$ , for  $\mu$ , *P* and  $M_{\langle ik \rangle}$ 

$$\begin{split} \mu &= \mu^{(0)} \left[ 1 - \frac{\pi^2}{12} \kappa (D-2) \left( \frac{k_B T}{\mu^{(0)}} \right)^2 \right] \tag{51} \\ &+ \frac{D-2}{3D} \left[ Q_D^I + \frac{\pi^2}{12} \kappa \left( \frac{k_B T}{\mu^{(0)}} \right)^2 Q_D^{II} \right] + O(\hbar^4) \,, \\ P &= \nu_E n^{(D+2)/D} \left[ 1 + \frac{\pi^2}{12} \kappa (D+2) \left( \frac{k_B T}{\mu^{(0)}} \right)^2 \right] \tag{52} \\ &+ n \left[ Q_E^I + \frac{\pi^2}{18} \kappa (D-2) \left( \frac{k_B T}{\mu^{(0)}} \right)^2 Q_E^{II} \right] + O(\hbar^4) \,, \\ M_{\langle ik \rangle} &= \mathcal{M}_{\langle ik \rangle}^I - \frac{\pi^2}{12} \kappa (D-2) \left( \frac{k_B T}{\mu^{(0)}} \right)^2 \mathcal{M}_{\langle ik \rangle}^{II} \,, \end{aligned}$$

with the quantum nonlocal-gradient second corrections  $Q_D^{II}$ ,  $Q_E^{II}$  and  $\mathcal{M}_{\langle ik \rangle}^{II}$  explicitly given in Eqs. (65)-(67) of Appendix.

In conclusion, by knowing  $M_{\langle ik \rangle}$  and P and using Eq. (38), the system (37) is explicitly closed. However, by indicating with  $\{\mu^{(c)}, P^{(c)}\}$  and  $\{\mu^{(q)}, P^{(q)}\}$  the classic and the quantum part of the chemical potential and pressure, as reported respectively in Eqs. (42)-(43), (45)-(46), (48)-(49) and (51)-(52), the spatial derivative of  $M_{ik}$  can be expressed in the following general form

$$\frac{\partial M_{ik}}{\partial x_k} = \frac{1}{m} \left\{ -\frac{\hbar^2}{12} \mathcal{T}_{ip} \frac{\partial}{\partial x_k} \left[ \left( \frac{\partial \mu^{(c)}}{\partial n} \right)^{-1} \mathcal{T}_{pk} \right] + \frac{\partial P^{(c)}}{\partial x_i} + n \frac{\partial \mu^{(q)}}{\partial x_i} \right\} + O(\hbar^4).$$
(54)

The relation above is a fourth major result. Indeed, in all cases (high and/or low temperature) and for any statistical approximation (i.e. different order of expansion), Eq. (54) represents a *general closure property* [45] for the quantum drift-diffusion system in Eq. (37).

We remark, that since many years the nonlocal gradient corrections have been extensively tested in real applications such as: atomic, surface, nuclear physics and electronic properties of clusters [46]. Analogously, density gradient expansions have been used to describe capture confinement and tunnelling processes for devices in the deca-nanometer regime, by showing a very good agreement both with available experiments and other microscopic methods [47]. The novelty of the present approach allows one to describe the Wigner gradient expansions in the framework of FES, by including also the vorticity. Consequently, the major results outlined above can have relevant applications in quantum turbulence, quantum fluids, quantized vortices, nanostructures, nanowires, thin layers and, by including also gradient thermal corrections, in graphene quantum transport [48]. Finally, we stress that Monte Carlo (MC) simulations and measurements of the thermodynamic properties of quantum gases, including energy, chemical potential, sound velocity and entropy, have been explored and compared recently [49]. In some cases these results have been interpreted in the framework of FES behaviour [50]. Similar measurements and MC simulations may be thought also in the presence of strong spatial inhomogeneous conditions and tested within the present nonlocal FES strategy. Accordingly, the QMEP including fractional exclusion statistics is here asserted as the fundamental principle of quantum statistical mechanics.

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### Appendix

Being  $w^{(0)}(\xi)$  solution of (30) (with  $\xi = e^{\alpha + x^2}$ ) we define the integrals

$$I_n(\alpha,\kappa) = \int_0^{+\infty} \frac{x^n}{w^{(0)}(e^{\alpha+x^2}) + \kappa} \, dx, \tag{55}$$

where, for n < 0, all the integral functions  $I_n(\alpha, \kappa)$  can be obtained by means of the following general differentiation property

$$\frac{\partial^r I_n}{\partial \alpha^r} = (-1)^r \left[ \frac{\Gamma\left(\frac{n+1}{2}\right)}{\Gamma\left(\frac{n+1}{2}-r\right)} \right] I_{n-2r}.$$
 (56)

The functions  $\eta_{ii}^{(s)}$ , contained in (39)-(40), are given by

$$\eta_{ij}^{(s)} = (-1)^i 2^{j-1} \frac{\Gamma\left(\frac{D}{2} + s + j - 1\right)}{\Gamma\left(\frac{D}{2} + s + i + j - 5\right)} \frac{I_{D+2(s+i+j)-11}}{I_{D+2s-1}}$$
(57)

and all nonlocal terms  $\{Q^{(q,p)}, Q_{\!\langle ik \rangle}\}$  are expressed by

$$Q^{(1,1)} = -\frac{2}{(D-2)^2} \left(\frac{I_{D-1}}{I_{D-3}}\right)^2 \left(\frac{\partial \ln n}{\partial x_k}\right)^2 + O(\hbar^2), \quad (58)$$

$$Q^{(1,2)} = \frac{1}{D(D-2)} \frac{I_{D-1}}{I_{D-3}} \left\{ \left[ 1 - \frac{D-4}{D-2} \frac{I_{D-1}}{I_{D-3}} \frac{I_{D-5}}{I_{D-3}} \right] \times \left( \frac{\partial \ln n}{\partial x_k} \right)^2 + \frac{\partial^2 \ln n}{\partial x_k \partial x_k} \right\} + \frac{1}{2D} \frac{m}{k_B T} \mathcal{T}_{ll}^2 + O(\hbar^2), \quad (59)$$

$$Q^{(2,1)} = \frac{3}{D-2} \frac{I_{D-1}}{I_{D-3}} \left\{ \left[ 1 - \frac{D-4}{D-2} \frac{I_{D-1}}{I_{D-3}} \frac{I_{D-5}}{I_{D-3}} \right] \right\}$$

$$\times \left(\frac{\partial \ln n}{\partial x_k}\right)^2 + \frac{\partial^2 \ln n}{\partial x_k \partial x_k} \bigg\} + \frac{3}{4} \frac{m}{k_B T} \mathcal{T}_{ll}^2 + \mathcal{O}(\hbar^2), \qquad (60)$$

$$Q_{\langle ij\rangle} = \frac{1}{D-2} \frac{I_{D-1}}{I_{D-3}} \left\{ \left[ 1 - \frac{D-4}{D-2} \frac{I_{D-1}}{I_{D-3}} \frac{I_{D-5}}{I_{D-3}} \right] \times \frac{\partial \ln n}{\partial x_{\langle i}} \frac{\partial \ln n}{\partial x_{j\rangle}} + \frac{\partial^2 \ln n}{\partial x_{\langle i} \partial x_{j\rangle}} \right\} + \frac{1}{2} \frac{m}{k_B T} \mathcal{T}_{\langle ij\rangle}^2 + \mathcal{O}(\hbar^2).$$
(61)

The quantum gradient corrections terms in (45)-(47) are

$$Q_B^{II} = \frac{\hbar^2}{4m} \left[ \frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \left( \frac{\partial \ln n}{\partial x_r} \right)^2 + \frac{m}{2} \frac{\mathcal{T}_{ll}^2}{k_B T} \right], \quad (62)$$
$$Q_C^{II} = \frac{\hbar^2}{12D} \frac{1}{m} \left[ 2D \frac{\partial^2 \ln n}{\partial x_r \partial x_r} + (3D-2) \left( \frac{\partial \ln n}{\partial x_r} \right)^2 \right]$$

$$+(D+4)\frac{m}{2}\frac{T_{ll}^2}{k_BT}$$
, (63)

$$M_{\langle ik\rangle}^{II} = -\frac{\hbar^2}{12} \frac{n}{m^2} \left[ \frac{\partial \ln n}{\partial x_{\langle i}} \frac{\partial \ln n}{\partial x_{j\rangle}} - \frac{m}{k_B T} T_{\langle ik\rangle}^2 \right], \tag{64}$$

The quantum gradient corrections terms in (51)-(53) are

$$Q_D^{II} = -\frac{\hbar^2}{2D} \frac{1}{m} \left[ 2D \frac{\partial^2 \ln n}{\partial x_r \partial x_r} + (D-4) \left( \frac{\partial \ln n}{\partial x_r} \right)^2 \right] + \frac{\hbar^2}{32} D(D-6) \frac{\mathcal{I}_{ll}^2}{\mu^{(0)}},$$
(65)

$$Q_E^{II} = -\frac{\hbar^2}{2D} \frac{1}{m} \left[ \frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \frac{(D-3)}{D} \left( \frac{\partial \ln n}{\partial x_r} \right)^2 \right] - \frac{\hbar^2}{32} \frac{\mathcal{T}_{ll}^2}{\mu^{(0)}}, (66)$$
$$\mathcal{M}_{\langle ik \rangle}^{II} = -\frac{\hbar^2}{12} \frac{n}{m^2} \left[ \frac{4}{D} \frac{\partial \ln n}{\partial x_{\langle i}} \frac{\partial \ln n}{\partial x_{\langle i}} + \frac{m}{2} \frac{D}{\mu^{(0)}} \mathcal{T}_{\langle ik \rangle}^2 \right], (67)$$