Quantum Maximum Entropy Principle for Fractional Exclusion Statistics

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Using the Wigner representation, compatibly with the uncertainty principle, we formulate a quantum maximum entropy principle for the fractional exclusion statistics. 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. Gradient quantum corrections are explicitly given at different levels of degeneracy and classical results are recovered when $\hbar \to 0$.

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The maximum entropy principle (MEP) is a pillar of classical statistical mechanics since it provides the basis for a rigorous formulation of any hydrodynamic model for a given physical system. The quantum extension of MEP (QMEP) is a major subject challenged a broad scientific community (including mathematicians, chemists, etc.) since 1957 [1,2]. Recently, a comprehensive review on QMEP was presented in Ref. [3]. Accordingly, all the results available from the literature for a Fermi and/or Bose gas have been generalized in the framework of a nonlocal Wigner theory [2,3].

Whereas fermions and bosons can exist in all dimensions, some low-dimensional systems exhibit elementary excitations that obey quantum statistics interpolating between fermionic and bosonic behaviors. In particular, the concept of anyons [4,5] is specific to two dimensions (2D) being connected to the braid group structure of particle trajectories [4,5], and the fractional statistics are parametrized by a phase factor that describes the particle exchange procedure in the configuration space [5]. In 2D systems, the fractional statistics was successfully applied to describe the fractional quantum Hall effect [6] and, more recently, direct evidence of fractional exchange phase factor was observed in experiments [7]. The fractional anyon statistics has also been formalized to some extent [8] in many one-dimensional (1D) models [9–13]. Accordingly, also in this case, anyons acquire a step-functionlike phase when two identical particles exchange their positions in a scattering process. 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 [5,14,15]

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

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

where $q(\mathbf{r}, \mathbf{r}') = q^{-1}(\mathbf{r}', \mathbf{r})$ [with $q(\mathbf{r}, \mathbf{r}) = \pm 1$] is a discontinuous function of its arguments [5,15] corresponding to a phase factor that denotes the system statistics [16].

A different notion of fractional statistics was introduced by Haldane [17] in arbitrary dimensions D. Quasiparticles that obey the fractional exclusion statistics (FES) are called "exclusons" with statistics (for a single specie) parameter $\kappa = -\delta G/\delta N$, where δG describes the change in size of the subset of available single-particle states corresponding to a variation of δN particles. It is known that FES is, in general, different from anyon statistics. Indeed, the exclusion statistics is assigned to elementary excitations of condensed-matter systems, which are not necessarily connected with braiding considerations [8,17]. However, there are some systems where a thermodynamics coincidence of the two statistics was shown [9,12,17,18].

The aim of this work is to consider anyonic systems satisfying FES, 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.

The theoretical formulation considers N identical anyons, and introduces in Fock space the statistical density-matrix ρ for the whole system, with $\mathrm{Tr}(\rho) = 1$ and the general Hamiltonian $H = \int d^D r \Psi^\dagger(\mathbf{r})[-\hbar^2/2m\nabla^2 + U(\mathbf{r})]\Psi(\mathbf{r}) + (1/2)\iint d^D r d^D r' \Psi^\dagger(\mathbf{r})\Psi^\dagger(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\Psi(\mathbf{r}') \times \Psi(\mathbf{r})$, 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, and Ψ and $\Psi^\dagger$ are the wave field operators satisfying the anyon relations Eqs. (1) and (2) with their properties [16]. Analogously, in the coordinate space representation, we define the reduced density matrix [2,3] of single particle $\langle \mathbf{r}|\hat{\varrho}|\mathbf{r}'\rangle = \langle \Psi^\dagger(\mathbf{r}')\Psi(\mathbf{r})\rangle = \mathrm{Tr}[\rho\Psi^\dagger(\mathbf{r}')\Psi(\mathbf{r})]$ that in an arbitrary representation takes the form $\langle \nu|\hat{\varrho}|\nu'\rangle = \langle a^\dagger_{\nu'} a_\nu\rangle = \mathrm{Tr}(\rho a^\dagger_{\nu'} a_\nu)$ where ν, ν' are the single-particle states, a_ν, $a^\dagger_{\nu'}$ are the annihilation and creation operators for these states, and $\langle \cdots \rangle$ is the statistical mean value. Then, we define the reduced Wigner function $\mathcal{F}_\mathcal{W} = (2\pi\hbar)^{-D}\int d^D\tau e^{-\frac{i}{\hbar}\tau\cdot\mathbf{p}}\langle\Psi^\dagger(\mathbf{r}-\tau/2)\Psi(\mathbf{r}+\tau/2)\rangle$ with the condition $\mathrm{Tr}(\hat{\varrho}) = \iint d^D r d^D p \mathcal{F}_\mathcal{W} = N$. Accordingly, by considering an operator of single particle $\hat{\mathcal{M}}(\hat{\mathbf{r}}, \hat{\mathbf{p}})$, we look for a function $\tilde{\mathcal{M}}(\mathbf{r}, \mathbf{p})$ in phase space that corresponds to operator $\hat{\mathcal{M}}$ introducing the Weyl-Wigner transform [2,3] $\mathcal{W}(\hat{\mathcal{M}}) = \tilde{\mathcal{M}}(\mathbf{r}, \mathbf{p})$, and analogously we define the inverse Weyl-Wigner transform [2,3] $\mathcal{W}^{-1}(\tilde{\mathcal{M}}) = \langle \mathbf{r}|\hat{\mathcal{M}}|\mathbf{r}'\rangle$ which maps the function $\tilde{\mathcal{M}}$ in phase space into the operator $\hat{\mathcal{M}}$ in Hilbert space.

Making use of quantum mechanics in second quantization form, within the generalized Hartree approximation [2,3] we obtain the evolution equation

$$i\hbar\frac{\partial}{\partial t}\langle \mathbf{r}|\hat{\varrho}|\mathbf{r}'\rangle = \int d^D r''[\langle \mathbf{r}|\hat{\mathcal{H}}|\mathbf{r}''\rangle\langle \mathbf{r}''|\hat{\varrho}|\mathbf{r}'\rangle - \langle \mathbf{r}|\hat{\varrho}|\mathbf{r}''\rangle\langle \mathbf{r}''|\hat{\mathcal{H}}|\mathbf{r}'\rangle], \tag{3}$$

where $\hat{\mathcal{H}} = \langle \mathcal{H}\rangle$ is the single-particle Hamiltonian operator with $\mathcal{H}(\mathbf{r}) = -\hbar^2/2m\nabla^2 + U(\mathbf{r}) + \int d^D r' \Psi^\dagger(\mathbf{r}')\times V(\mathbf{r}, \mathbf{r}')\Psi(\mathbf{r}')$.

Accordingly, following a usual script [2,3], we obtain the full gradient expansion of the Wigner equation

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

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

To take into account *ab initio* the FES, we evaluate the entropy [19] S for a noninteracting system under nonequilibrium conditions in terms of the occupation numbers

$$S = -k_B\sum_\nu y\{\langle \bar{N}_\nu\rangle \ln\langle \bar{N}_\nu\rangle + (1-\kappa\langle \bar{N}_\nu\rangle)\ln(1-\kappa\langle \bar{N}_\nu\rangle) - [1+(1-\kappa)\langle \bar{N}_\nu\rangle]\ln[1+(1-\kappa)\langle \bar{N}_\nu\rangle]\}$$

with k_B the Boltzmann constant, $\langle \bar{N}_\nu\rangle = \langle a_\nu^\dagger a_\nu\rangle/y$, y the spin degeneration, and κ the statistical parameter of fractional statistics. If we consider the Schrödinger equation for the single-particle Hamiltonian $\hat{\mathcal{H}}$, then the occupation numbers $\langle N_\nu\rangle$ associated with the energies E_ν will completely specify the gas macroscopic state. In particular, using Eq. (3) in stationary conditions, both $\hat{\varrho}$ and any operator $\hat{\Phi}(\hat{\varrho})$ are diagonal in the base $|\nu\rangle$. Therefore, by introducing as a function of $\hat{\varrho}$

$$\hat{\Phi}(\hat{\varrho}) = y\left\{\frac{\hat{\varrho}}{y}\ln\left(\frac{\hat{\varrho}}{y}\right) + \left(\hat{I} - \kappa\frac{\hat{\varrho}}{y}\right)\ln\left(\hat{I} - \kappa\frac{\hat{\varrho}}{y}\right) - \left[\hat{I} + (1-\kappa)\frac{\hat{\varrho}}{y}\right]\ln\left[\hat{I} + (1-\kappa)\frac{\hat{\varrho}}{y}\right]\right\} \tag{5}$$

with $\hat{I}$ the identity, the quantum entropy for an excluson gas can be described in terms of the following functional of the reduced density operator

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

By introducing a set $\mathcal{N}$ of single-particle observables $\{\hat{\mathcal{M}}_A\}$ and the corresponding space phase functions $\{\tilde{\mathcal{M}}_A\}$, we define the local moments $M_A(\mathbf{r}, t) = \int d^D p \tilde{\mathcal{M}}_A(\mathbf{r}, \mathbf{p})\times \mathcal{F}_{\mathcal{W}}(\mathbf{r}, \mathbf{p}, t)$ and we use the functional Eq. (6) as an informational entropy of the system. Thus, we consider the new global functional [2,3]

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

as being $\tilde{\lambda}_A(\mathbf{r}, t)$ the nonlocal Lagrange multipliers.

The solution of the constraint $\delta\tilde{S} = 0$ implies

$$\hat{\varrho} = y\{\hat{w}(\hat{\xi}) + \kappa\hat{I}\}^{-1} \tag{8}$$

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

$$[\hat{w}(\hat{\xi})]^\kappa[\hat{I} + \hat{w}(\hat{\xi})]^{1-\kappa} = \hat{\xi} \tag{9}$$

with the operator

$$\hat{\xi} = \exp\left[\mathcal{W}^{-1}\left(\sum_{A=1}^{\mathcal{N}}\lambda_A\tilde{\mathcal{M}}_A\right)\right] \quad \text{and} \quad \lambda_A = \frac{\tilde{\lambda}_A}{k_B}. \tag{10}$$

The set of Eqs. (8)–(10) is the first major result. It generalizes existing results [19], in an operatorial sense, under both thermodynamic equilibrium and nonequilibrium conditions. Accordingly, for any fixed number $\mathcal{N}$ of moments M_A, we can consider a consistent expansion around $\hbar$ of the Wigner function. In this way we separate classical from quantum nonlocal dynamics, and obtain order-by-order gradient correction terms. In particular, one can prove that $\tilde{w} = \mathcal{W}(\hat{w})$, $\mathcal{F}_{\mathcal{W}}$, and the moments M_A can be expanded in power of $\hbar$ as

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

To this purpose, the Lagrange multipliers λ_A must be determined by inverting, order by order, the constraints $M_A = (2\pi\hbar)^{-D}\int d^D p\tilde{\mathcal{M}}_A\mathcal{W}(\hat{\varrho}[\lambda_B(\mathbf{r}, t), \tilde{\mathcal{M}}_B])$, where the inversion problem can be solved [2,3] only by assuming that also the Lagrange multipliers admit for an expansion in even powers of $\hbar$, $\lambda_A = \lambda_A^{(0)} + \sum_{k=1}^{\infty}\hbar^{2k}\lambda_A^{(2k)}$. By using Eqs. (8)–(10) we further succeed in determining the following expression for the reduced Wigner function:

$$\mathcal{F}_{\mathcal{W}} = \frac{\tilde{y}}{w^{(0)}(\xi) + \kappa}\left\{1 + \sum_{r=1}^{\infty}\hbar^{2r}\mathcal{P}_{2r}\right\}, \tag{11}$$

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

$$[w^{(0)}(\xi)]^\kappa[1 + w^{(0)}(\xi)]^{1-\kappa} = \xi. \tag{12}$$

Equation (11) is the second major result. Indeed, making use of $\xi_0 = e^{\Pi_0}$ with $\Pi_0 = \sum \lambda_A^{(0)}\tilde{\mathcal{M}}_A$, from Eq. (11) we obtain, explicitly, the first order ($r = 1$) quantum correction

$$\mathcal{P}_2=\left\{\frac{2}{[w^{(0)}(\xi_0)+\kappa]^2}\left(\xi_0\frac{dw^{(0)}}{d\xi_0}\right)^2-\frac{1}{w^{(0)}(\xi_0)+\kappa}\left[\xi_0^2\frac{d^2w^{(0)}}{d\xi_0^2}+\xi_0\frac{dw^{(0)}}{d\xi_0}\right]\right\}\mathcal{H}_2^{(2)}-\left\{\frac{6}{[w^{(0)}(\xi_0)+\kappa]^2}\left[\frac{1}{w^{(0)}(\xi_0)+\kappa}\left(\xi_0\frac{dw^{(0)}}{d\xi_0}\right)^3\right.\right.$$
$$\left.\left.-\left(\xi_0\frac{dw^{(0)}}{d\xi_0}\right)^2-\xi_0^3\frac{d^2w^{(0)}}{d\xi_0^2}\frac{dw^{(0)}}{d\xi_0}\right]+\frac{1}{w^{(0)}(\xi_0)+\kappa}\left[\xi_0^3\frac{d^3w^{(0)}}{d\xi_0^3}+3\xi_0^2\frac{d^2w^{(0)}}{d\xi_0^2}+\xi_0\frac{dw^{(0)}}{d\xi_0}\right]\right\}\mathcal{H}_3^{(2)} \tag{13}$$

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

$$\mathcal{H}_3^{(2)}=-\frac{1}{24}\left[\frac{\partial^2\Pi_0}{\partial x_i\partial x_j}\frac{\partial\Pi_0}{\partial p_i}\frac{\partial\Pi_0}{\partial p_j}+\frac{\partial^2\Pi_0}{\partial p_i\partial p_j}\frac{\partial\Pi_0}{\partial x_i}\frac{\partial\Pi_0}{\partial x_j}-2\frac{\partial^2\Pi_0}{\partial x_i\partial p_j}\frac{\partial\Pi_0}{\partial x_j}\frac{\partial\Pi_0}{\partial p_i}\right], \tag{14}$$

$$\mathcal{H}_2^{(2)}=-\frac{1}{8}\left[\frac{\partial^2\Pi_0}{\partial x_i\partial x_j}\frac{\partial^2\Pi_0}{\partial p_i\partial p_j}-\frac{\partial^2\Pi_0}{\partial x_i\partial p_j}\frac{\partial^2\Pi_0}{\partial x_j\partial p_i}\right]. \tag{15}$$

We remark on the following points: (i) For $\kappa=1$ and $\kappa=0$ we recover the gradient nonlocal results obtained for Fermi and Bose gases [2,3]. (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 [20]. (iii) In thermodynamics equilibrium conditions we can write $\Pi|_E=\alpha+\beta\tilde{\varepsilon}$ where $\tilde{\varepsilon}=m\tilde{u}^2/2$, with $\tilde{u}_i=u_i-\lambda_i$ the peculiar velocity, $u_i=p_i/m$ the group velocity, and $\{\alpha,\beta,\lambda_i\}$ the equilibrium nonlocal Lagrange multipliers.

As relevant application of the above results, we consider an excluson gas in isothermal equilibrium conditions. Accordingly, $\beta=(k_BT)^{-1}$, 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 $v_i(\mathbf{r},t)=n^{-1}\int d^Dpu_i\mathcal{F}_{\mathcal{W}}$. In this case it is necessary to determine a closed set of balance equations for the variables $\{n,v_i\}$. Thus, by considering the kinetic fields $\{1,u_i\}$ and using Eq. (4) we obtain the quantum drift-diffusion model [2]

$$\dot{n}+n\frac{\partial v_k}{\partial x_k}=0,\qquad \dot{v}_i+\frac{1}{n}\frac{\partial M_{ik}}{\partial x_k}+\frac{1}{m}\frac{\partial V_{\rm eff}}{\partial x_i}=0, \tag{16}$$

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

$$M_{ik}=M_{\langle ik\rangle}+\frac{P}{m}\delta_{ik}+\mathcal{O}(\hbar^4) \tag{17}$$

with the traceless part $M_{\langle ik\rangle}+\mathcal{O}(\hbar^4)=\int d^Dp\tilde{u}_{\langle i}\tilde{u}_{k\rangle}\mathcal{F}_{\mathcal{W}}|_E$ and the quantum pressure $P+\mathcal{O}(\hbar^4)=2/D\int d^Dp\tilde{\varepsilon}\mathcal{F}_{\mathcal{W}}|_E$ independent constitutive quantities. Then, by making use of Eqs. (11)–(15) we can calculate the variables $\{n,P,M_{\langle ik\rangle}\}$ by determining the general relations

$$I_{D-1}(\alpha,\kappa)=\gamma\frac{n}{T^{D/2}}\left\{1-\frac{\hbar^2}{12m}\frac{1}{k_BT}\left[\sum_{p=1}^{2}\eta_{1p}^{(0)}\mathcal{Q}^{(1,p)}+\eta_{21}^{(0)}\mathcal{Q}^{(2,1)}\right]\right\}+\mathcal{O}(\hbar^4), \tag{18}$$

$$P=\frac{2}{D}nk_BT\frac{I_{D+1}}{I_{D-1}}\left\{1+\frac{\hbar^2}{12m}\frac{1}{k_BT}\left[\sum_{p=1}^{2}(\eta_{1p}^{(1)}-\eta_{1p}^{(0)})\mathcal{Q}^{(1,p)}+(\eta_{21}^{(1)}-\eta_{21}^{(0)})\mathcal{Q}^{(2,1)}\right]\right\}+\mathcal{O}(\hbar^4), \tag{19}$$

$$M_{\langle ik\rangle}=-\frac{\hbar^2}{12}\frac{n}{m^2}(D-2)\frac{I_{D-3}}{I_{D-1}}\mathcal{Q}_{\langle ik\rangle}+\mathcal{O}(\hbar^4), \tag{20}$$

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 $\{\mathcal{Q}^{(q,p)},\mathcal{Q}_{\langle ik\rangle}\}$ are explicitly given in Appendix A.

Equations (18)–(20) constitute the third major result. In particular, by Eq. (18) we can determine the generalized quantum chemical potential $\mu=-\alpha k_BT$, and by using Eq. (19) we obtain the generalized quantum equation of state. Thus, by introducing the usual Bohm quantum potential $Q_B=-(\hbar^2/2m\sqrt{n})\triangle\sqrt{n}$ and the vorticity tensor $\mathcal{T}_{ij}=(\partial v_i/\partial x_j-\partial v_j/\partial x_i)$, the following analytical cases are analyzed under isothermal equilibrium condition.

High-temperature and/or low-density limits.—First approximation: By using the first term of a series expansion [21] for the functions $I_n(\alpha,\kappa)$, we obtain the Boltzmann limit, which is independent from κ, as being $I_n(\alpha)\approx(1/2)\Gamma[(n+1)/2]\exp(-\alpha)$. Thus, by defining the quantity $\chi^{(0)}=y^{-1}[(2\pi\hbar^2)/(mk_B)]^{D/2}(n/T^{D/2})$ and using Eqs. (18)–(20) we obtain the generalized expressions

$$\mu=k_BT\ln[\chi^{(0)}]+\frac{Q_B^I}{3}+\mathcal{O}(\hbar^4),\qquad P=nk_BT+nQ_C^I+\mathcal{O}(\hbar^4), \tag{21}$$

with the first quantum nonlocal gradient corrections

$$Q_B^I=Q_B-\frac{\hbar^2}{16}\frac{\mathcal{T}_{ll}^2}{k_BT},\qquad Q_C^I=-\frac{\hbar^2}{12D}\frac{1}{m}\left[\frac{\partial^2\ln n}{\partial x_r\partial x_r}+\frac{m}{k_BT}\mathcal{T}_{ll}^2\right],$$

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

$$M_{\langle ik\rangle}^I=-\frac{\hbar^2}{12}\frac{n}{m^2}\left[\frac{\partial^2\ln n}{\partial x_{\langle i}\partial x_{k\rangle}}+\frac{m}{k_BT}\mathcal{T}_{\langle ik\rangle}^2\right]+\mathcal{O}(\hbar^4). \tag{22}$$

By neglecting vorticity effects ($\mathcal{T}_{ik} = 0$) we recover well-known relations [2,3,22], while by including vorticity terms we reobtain some recent results for a quantum Boltzmann gas [23].

Second approximation: By using the first two terms of the series expansion [21] with a standard iterative procedure [2,3], we determine the correct second quantum statistical approximation in terms of the quantity $\chi^{(0)} \ll 1$ as being

$$\mu = k_B T \ln\left[\left(1 + \frac{2\kappa - 1}{2^{D/2}}\chi^{(0)}\right)\chi^{(0)}\right] + \frac{1}{3}\left(Q_B^I + \frac{2\kappa - 1}{2^{D/2}}\chi^{(0)} Q_B^{II}\right) + \mathcal{O}(\hbar^4), \qquad (23)$$

$$P = nk_B T\left(1 + \frac{2\kappa - 1}{2^{D/2+1}}\chi^{(0)}\right) + n\left(Q_C^I + \frac{2\kappa - 1}{2^{D/2+1}}\chi^{(0)} Q_C^{II}\right) + \mathcal{O}(\hbar^4), \qquad (24)$$

$$M_{\langle ik\rangle} = M_{\langle ik\rangle}^I + \frac{2\kappa - 1}{2^{D/2}}\chi^{(0)} M_{\langle ik\rangle}^{II} + \mathcal{O}(\hbar^4), \qquad (25)$$

with the second quantum nonlocal gradient corrections Q_B^{II}, Q_C^{II}, and $M_{\langle ik\rangle}^{II}$ explicitly given in Appendix A.

Low-temperature limits.—Under strong degeneracy, we make use of an asymptotic expansion [21] 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 $\nu_E = [4\pi/(D+2)](\hbar^2/m)[(\kappa/y)\times\Gamma(D/2+1)]^{2/D}$ and $\mu^{(0)} = [(D+2)/2]\nu_E n^{2/D}$, for μ and P we obtain

$$\mu = \mu^{(0)} + \frac{D-2}{3D} Q_D^I + \mathcal{O}(\hbar^4), \qquad (26)$$

$$P = \nu_E n^{(D+2)/D} + n Q_E^I + \mathcal{O}(\hbar^4), \qquad (27)$$

with the first quantum nonlocal gradient 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 $\mathcal{M}_{\langle ik\rangle}^I$ for the tensor $M_{\langle ik\rangle}$

$$\mathcal{M}_{\langle ik\rangle}^I = -\frac{\hbar^2}{12}\frac{n}{m^2}\left[\frac{\partial^2 \ln n}{\partial x_{\langle i}\partial x_{k\rangle}} + \frac{2}{D}\frac{\partial \ln n}{\partial x_{\langle i}}\frac{\partial \ln n}{\partial x_{k\rangle}} + \frac{m}{2}\frac{D}{\mu^{(0)}}\mathcal{T}_{\langle ik\rangle}^2\right] + \mathcal{O}(\hbar^4). \qquad (28)$$

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 the Thomas-Fermi-Weizsacker theory [2,3,24]. For $\kappa \neq 1$, and by including also the vorticity terms, we generalize these results to excluson gases in the low-temperature limit.

Second approximation: By considering the first two terms of the asymptotic expansion in series [21] we obtain the correct second quantum statistical approximation in terms of the quantities $(k_B T/\mu^{(0)})^2 \ll 1$, for μ, P and $M_{\langle ik\rangle}$

$$\mu = \mu^{(0)}\left[1 - \frac{\pi^2}{12}\kappa(D-2)\left(\frac{k_B T}{\mu^{(0)}}\right)^2\right] + \frac{D-2}{3D}\left[Q_D^I + \frac{\pi^2}{12}\kappa\left(\frac{k_B T}{\mu^{(0)}}\right)^2 Q_D^{II}\right] + \mathcal{O}(\hbar^4), \qquad (29)$$

$$P = \nu_E n^{(D+2)/D}\left[1 + \frac{\pi^2}{12}\kappa(D+2)\left(\frac{k_B T}{\mu^{(0)}}\right)^2\right] + n\left[Q_E^I + \frac{\pi^2}{18}\kappa(D-2)\left(\frac{k_B T}{\mu^{(0)}}\right)^2 Q_E^{II}\right] + \mathcal{O}(\hbar^4), \qquad (30)$$

$$M_{\langle ik\rangle} = \mathcal{M}_{\langle ik\rangle}^I - \frac{\pi^2}{12}\kappa(D-2)\left(\frac{k_B T}{\mu^{(0)}}\right)^2 \mathcal{M}_{\langle ik\rangle}^{II}, \qquad (31)$$

with the second quantum nonlocal gradient corrections Q_D^{II}, Q_E^{II}, and $\mathcal{M}_{\langle ik\rangle}^{II}$ explicitly given in Appendix A.

In conclusion, knowing $M_{\langle ik\rangle}$ and P and using Eq. (17), the system in Eq. (16) is 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, the spatial derivative of M_{ik} can be expressed in the general form

$$\frac{\partial M_{ik}}{\partial x_k} = \frac{1}{m}\left\{-\frac{\hbar^2}{12}\mathcal{T}_{ip}\frac{\partial}{\partial x_k}\left[\left(\frac{\partial \mu^{(c)}}{\partial n}\right)^{-1}\mathcal{T}_{pk}\right] + \frac{\partial P^{(c)}}{\partial x_i} + n\frac{\partial \mu^{(q)}}{\partial x_i}\right\} + \mathcal{O}(\hbar^4). \qquad (32)$$

The relation above is the fourth major result. Indeed, in all cases (high and/or low temperature) and for any statistical approximation Eq. (32) represents a general closure property for the quantum drift-diffusion system in Eq. (16).

We remark that for many years the nonlocal gradient corrections have been extensively tested in real applications such as atomic, surface, nuclear physics, and electronic properties of clusters [24]. Analogously, density gradient expansions have been used to describe capture confinement and tunnelling processes for devices in the decananometer regime by showing a very good agreement both with available experiments and other microscopic methods [25]. 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 [26]. Accordingly, the QMEP including FES is here asserted as the fundamental principle of quantum statistical mechanics.

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APPENDIX A

With $w^{(0)}(\xi)$ being the solution of Eq. (12) (with $\xi = e^{\alpha+x^2}$) we define the integrals $I_n(\alpha,\kappa) = \int_0^{+\infty} x^n \times [w^{(0)}(e^{\alpha+x^2})+\kappa]^{-1}dx$, where for $n<0$, all the integral functions $I_n(\alpha,\kappa)$ can be obtained by means of the following general differentiation property: $\partial^r I_n/\partial\alpha^r = (-1)^r[\Gamma(\frac{n+1}{2})/\Gamma(\frac{n+1}{2}-r)]I_{n-2r}$.

Functions $\eta_{ij}^{(s)}$ in Eqs. (18) and (19) are given by

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

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

$$\mathcal{Q}^{(1,1)} = -\frac{2}{(D-2)^2}\left(\frac{I_{D-1}}{I_{D-3}}\right)^2\left(\frac{\partial \ln n}{\partial x_k}\right)^2 + \mathcal{O}(\hbar^2), \quad \text{(A1)}$$

$$\mathcal{Q}^{(1,2)} = \frac{1}{D(D-2)}\frac{I_{D-1}}{I_{D-3}}\left\{\left[1-\frac{D-4}{D-2}\frac{I_{D-1}}{I_{D-3}}\frac{I_{D-5}}{I_{D-3}}\right]\left(\frac{\partial \ln n}{\partial x_k}\right)^2 + \frac{\partial^2 \ln n}{\partial x_k \partial x_k}\right\} + \frac{1}{2D}\frac{m}{k_B T}\mathcal{T}_{ll}^2 + \mathcal{O}(\hbar^2), \quad \text{(A2)}$$

$$\mathcal{Q}^{(2,1)} = 3D\mathcal{Q}^{(1,2)} - \frac{3}{4}\frac{m}{k_B T}\mathcal{T}_{ll}^2 + \mathcal{O}(\hbar^2), \quad \text{(A3)}$$

$$\mathcal{Q}_{\langle ij\rangle} = \frac{1}{D-2}\frac{I_{D-1}}{I_{D-3}}\left\{\left[1-\frac{D-4}{D-2}\frac{I_{D-1}}{I_{D-3}}\frac{I_{D-5}}{I_{D-3}}\right]\frac{\partial \ln n}{\partial x_{\langle i}}\frac{\partial \ln n}{\partial x_{j\rangle}} + \frac{\partial^2 \ln n}{\partial x_{\langle i}\partial x_{j\rangle}}\right\} + \frac{1}{2}\frac{m}{k_B T}\mathcal{T}_{\langle ij\rangle}^2 + \mathcal{O}(\hbar^2). \quad \text{(A4)}$$

The gradient corrections terms in Eqs. (23)–(25) are

$$Q_B^{II} = \frac{\hbar^2}{4m}\left[\frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \left(\frac{\partial \ln n}{\partial x_r}\right)^2 + \frac{m}{2}\frac{\mathcal{T}_{ll}^2}{k_B T}\right],$$

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

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

The gradient corrections terms in Eqs. (29)–(31) are

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

$$Q_E^{II} = -\frac{\hbar^2}{2D}\frac{1}{m}\left[\frac{\partial^2 \ln n}{\partial x_r \partial x_r} + \frac{(D-3)}{D}\left(\frac{\partial \ln n}{\partial x_r}\right)^2\right] - \frac{\hbar^2}{32}\frac{\mathcal{T}_{ll}^2}{\mu^{(0)}},$$

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

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