A Nonlocal Formulation of Quantum Maximum Entropy Principle Including Fractional Exclusion Statistics

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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 Γ 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], [2]; 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], [3]. In particular, by introducing the principle of maximum entropy (MEP) it was found possible to derive rigorous hydrodynamic (HD) models based on the *moments* of the distribution function to all orders of a power expansion and including appropriate closure conditions [4], [5]. 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 [3], [6], 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. Fron 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, quantum turbulence, quantum fluids, quantized vortices, nuclear physics, confined carrier transport in semiconductor heterostrucures, phonon and electron transport in nanostructures, nanowires and thin layers.

The aim of this talk is to address the above drawbacks by defining a quantum entropy in terms of the *reduced density matrix*, thus explicitly incorporating quantum statistics into problems involving a system of identical particles. As a further step, with respect to the uncertainty principle, starting from the Wigner representation we formulate a quantum maximum entropy principle which, in the framework of information theory, allows us to obtain a non-local theory for the system under study. As a final step, we determine a closed quantum hydrodynamic model for the macroscopic variables used as constraints in the QMEP approach.

THE NONLOCAL QMEP

By considering the Wigner formalism [7], the QMEP was asserted as the fundamental principle of quantum statistical mechanics when it becomes necessary to treat systems in partially specified quantum mechanical states [8]. Recently, in a series of papers [5], [8], [9] we have presented a set of results addressing this problem by emphasizing the role played by a proper formulation of a QMEP to close quantum hydrodynamic models

978-3-901578-26-7 © 2013 Society for Micro- and Nanoelectronics

in the framework of Extended Thermodynamics. Here, we present a rigorous nonlocal formulation of QMEP by including explicitly Fermi statistics, Bose statistics and, more generally, fractional exclusion statistics (FES).

Relevant results of the present investigation are:
(i) The development of a generalized quantum kinetic equation, in the mean field approximation, for the reduced Wigner function.
(ii) The construction of Extended Quantum Hydrodynamic models evaluated exactly to all orders of $\hbar$.
(iii) The definition of a generalized quantum entropy as global functional of the reduced density matrix.
(iv) The formulation of a quantum version of the maximum entropy principle obtained by determining an explicit functional form of the reduced density operator, which requires the consistent introduction of nonlocal quantum Lagrange multipliers within a Moyal expansion.
(v) The development of a quantum-closure procedure that, for a set of relevant quantum regimes, includes nonlocal statistical effects in the corresponding quantum hydrodynamic systems, both in thermodynamic equilibrium and nonequilibrium conditions.
(vi) The extension of QMEP in the framework of FES.
In particular, within point (vi) the anionic systems satisfying FES [9] are proven to generalize all the results available in the literature in terms of both the kind of statistics and the nonlocal description for excluson gases. Finally gradient quantum corrections are explicitly given at different levels of degeneracy, and classical results are recovered when $\hbar \to 0$.

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 [10]. 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 [11]. We conclude, that the novelty of the present approach allows one to describe the Wigner gradient expansions in the framework of quantum statistics by including also gradient thermal corrections and vorticity terms. As a consequence, the major results outlined above can have relevant applications in quantum turbulence, quantum fluids and quantized vortices. Accordingly, the QMEP including FES is here asserted as the most advanced formulation of the fundamental principle of quantum statistical mechanics.

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