

On the Nonequilibrium Statistical Operator and Classical Thermofield Dynamics

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A nonequilibrium statistical operator (NSO) is built for classical systems using a field theory in classical phase space, which is but a classical version of the thermofield dynamics formalism. The approach developed here starts with a second-quantized version of this phase-space field theory. Then elements of symmetry are analysed and invariants of the theory are introduced. The local conservation laws are derived and used to make explicit NSO. Such a method is applied to derive the Fokker-Planck-Kramers equation.

I. Introduction

In statistical mechanics a general and celebrated approach to treat nonequilibrium systems was proposed by Zubarev [1], the so-called nonequilibrium statistical operator (NSO), which is based in a generalization of the Gibbs ensemble concept.

The NSO formalism has been used to treat nonequilibrium situations, which can be classified in two general classes of phenomena, associated with the response of the system to mechanical perturbations, as well as to thermal perturbations. Such a formalism has been a powerful tool to treat experimental situations, with a particular emphasis to quantum systems. So, for instance, Buishvili et al [2]–[7] applied NSO to develop a diffusion theory for nuclear spin, to study magnetic resonance, and to analyze the dynamics of nuclear polarization in solids; Kalashnikov [8], in his turn, used such an approach to study relaxation process of spin lattices and hot electrons in semiconductors; Zubarev and Bashkurov [9, 10] derived equations of type Fokker-

Planck-Kramers. More recently, Tang [11] applied the method to deduce relations involving heat and work for out of equilibrium non-homogeneous systems. In particular, Professor Luzzi and collaborators [12]–[17] have developed the NSO concept, and have been successful, in a series of works, to describe photo-excited semiconductors in regions far from thermal equilibrium, and to derive kinetic equations. In a formal aspect, trying to improve the nonequilibrium theory to relativistic fields, Zubarev and Tokarchuk [18] have shown that NSO can be developed in the context of the called (quantum) thermofield dynamics [19, 20], an operator version of the Schwinger-Keldysh closed-time-path formalism.

For classical irreversible processes, NSO is based on the distribution function, that is the solution of the Liouville equation. Such a formulation has, as a basic characteristic, the fact that the (usual) Liouville equation describes the evolution of classical states with a fixed number of particles. This fact, in particular, makes difficult the use of the method where the number of particles is variable, as it is, for example, the case

when chemical reactions take place. On the other hand, despite the renewal interest in the relativistic classical kinetic theory, motivated by the use of such a theory to deal with the quark-gluons plasma formed during a heavy-ion collision [21], in the relativistic situation NSO is only partially developed [1]. These aspects show that the NSO approach for classical systems has not been fully developed and explored, in spite of the importance of a myriad of (relativistic or non relativistic) other classical systems, as the intracellular transport process, classical bidimensional plasmas, gases, and so on.

The main goal of this paper is to improve the NSO method for a broader set of classical systems. In order to do this, the NSO formalism is developed in the context of a classical version of thermofield dynamics approach and applied to derive a basic kinetic equation.

Through the analysis of representations of the Galilei group on Liouville spaces [22, 23], a classical counterpart of the (quantum) thermofield dynamics formalism [24, 25] was recently identified as the Schönberg's generalization of classical statistical mechanics [26, 27, 28]. This approach [29]–[39], based on the use of methods similar to those of second quantization but for the classical Liouville equation, is built through the notion of phase-space fields, say $\psi(x)$, $x = (q, p)$, satisfying commutation (anticommutation) rules, according to the bosonic (fermionic) nature of the classical particles. The operators $\psi(x)$ are defined in a Hilbert space (the Schönberg-Fock space), where the state of the system is established, and the usual theory is derived for a special class of Hermitian operators.

In such a phase-space field theory, that can also be considered as a second quantized version of the framework introduced by Prigogine and collaborators [35, 40, 41], some aspects should be pointed out: (i) The dynamical variables of a classical system are operators defined on Fock space. This fact allows a generalization of the concept of classical observable, by the introduction of quantities as, for instance, the “quantized” Liouville operator. (ii) The use of symmetrized or antisymmetrized Fock space allows us to introduce the indistinguishability of particles within the context of classical mechanics, solving, for example, the Gibbs paradox in classical statistical mechanics. (iii) As in the

case of a quantum field theory, the quanta of the field $\psi(x)$ are interpreted as the classical particles. (iv) The concept of grand-ensemble is introduced in a natural way.

The Schönberg's classical second-quantization formalism, with its associated representations, gives rise then to new aspects of the description of classical systems, as well as a new mathematical construction is introduced in classical statistical mechanics. In this realm, therefore, we can explore the notion of classical NSO, taking advantage of the vector space structure, early developed for quantum systems.

In order to go on with, a résumé of the classical second-quantization method on phase space is presented in Section II, with emphasis on some aspects which are relevant for the sequence of this work. Thus we show that for every additive variable defined in phase space, there exists an operator in the Schönberg-Fock space. Besides, in Section III, some elements of symmetry are studied, and the constants of motion are identified in terms of quantized field operators $\psi(x)$. In this context, we present the local conservation equations. Our NSO is introduced in Section IV, with a derivation of the Fokker-Planck-Kramers equation. This application has a twofold proposal. First, to show how such a NSO method works out in a specific situation. Second, as the derivation of such a kinetic equation is not a trivial problem, our method can be better compared with standard procedures. Section V is dedicated to concluding remarks.

II. Field Formalism in Phase Space

Consider a classical n -body system described by the Liouville equation

$$\partial_t f_n = \{h_n, f_n\}_n, \quad (1)$$

where

$$\begin{aligned} \{F, G\}_n &= \sum_{i=1}^n \left(\frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial G}{\partial q_i} \frac{\partial F}{\partial p_i} \right) \\ &\equiv \{F, \}_n G \end{aligned}$$

is the n -Poisson bracket;

$$\begin{aligned} h_n &= \sum_{i=1}^n \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq l=1}^n V(|q_i - q_l|) \\ &= h_{n,o} + h_{n,int}, \end{aligned} \quad (2)$$

is the Hamiltonian; p_l is the momentum of the particle whose position is q_l ; and $f_n = f(q_1, q_2, \dots, q_n, p_1, p_2, \dots, p_n; t)$ is the probability density in the phase space of the n -body system.

In the Schönberg's formalism, such a classical n -body system is described in terms of field operators $\psi(x; t)$ defined on phase space ($x = (q, p)$) and characterized by the commutation and anticommutation rules

$$[\psi(x; t), \psi^*(x'; t)]_{\pm} = \delta(x - x'), \tag{3}$$

$$[\psi(x; t), \psi(x'; t)]_{\pm} = [\psi^*(x; t), \psi^*(x'; t)]_{\pm} = 0, \tag{4}$$

where $\delta(x - x') = \delta(q - q')\delta(p - p')$, and $[A, B]_{\pm} = AB \pm BA$. In this approach, the equation of motion for the state of the system, $|\chi(t)\rangle$, is given by

$$i\partial_t |\chi(t)\rangle = L|\chi(t)\rangle, \tag{5}$$

where L is the "second-quantized" Liouville operator, that is

$$L = \int dx \psi^*(x; t)L_o\psi(x; t) + \frac{1}{2} \int dx dx' \psi^*(x; t)\psi^*(x'; t)L_{in}\psi(x'; t)\psi(x; t), \tag{6}$$

with $dx = dpdq$,

$$L_o = i\{h_o, \}_1 \equiv -i\frac{p}{m}\frac{\partial}{\partial q},$$

$$L_{in} = i\{h_{in}, \}_2 \equiv i\frac{\partial V(q, q')}{\partial q}\frac{\partial}{\partial p} + i\frac{\partial V(q, q')}{\partial q'}\frac{\partial}{\partial p'},$$

and $\psi^*(x; t)$ being the Hermitian conjugated of $\psi(x; t)$. $|\chi(t)\rangle$ is an element of the Fock space (the Schönberg-Fock space) $\mathcal{F}_i = \bigoplus_{n=0}^{\infty} \mathcal{F}_i^n$, $\mathcal{F}_i^n = \mathcal{H} \otimes_i \mathcal{H} \otimes_i \dots \otimes_i \mathcal{H}$ (n -factors), with $i = a, s$, such that $\otimes_{i=s}$ ($\otimes_{i=a}$) is a symmetrized (antisymmetrized) product, and \mathcal{H} is the Hilbert space introduced by Koopman[42]. The choice of sign in the rules (3) and (4) determines the space \mathcal{F}_s or \mathcal{F}_a to be used and the statistics of the particles, which here are considered indistinguishable.

The number operator is defined by

$$n = \int n(x, t)dx, \quad n(x, t) = \psi^*(x; t)\psi(x; t), \tag{7}$$

for which any of the eigenvalues $0, 1, 2, \dots$ may be assigned. In the space \mathcal{F}_i , a general state, solution of Eq.(5), is given by

$$|\chi(t)\rangle = \theta(t)|0\rangle + \sum_{n=1}^{\infty} \frac{1}{\sqrt{n!}} \int \theta(x_1, x_2, \dots, x_n; t)|\chi_n\rangle d^n x,$$

where $d^n x = dx_1 dx_2 \dots dx_n$, $|\chi_n\rangle = \psi^*(x_1; t)\psi^*(x_2; t)\dots\psi^*(x_n; t)|0\rangle$. The state $|0\rangle$, the vacuum defined in the phase space, is normalized, $\langle 0|0\rangle = 1$, and $\psi(x; t)|0\rangle = 0$. The coefficients

$$\theta(x_1, x_2, \dots, x_n; t) = \frac{1}{\sqrt{n!}} \langle 0 | \prod_{i=1}^n \psi(x_i; t) | \chi \rangle$$

are complex-valued functions, which belong to the class of functions $\mathcal{L}_2(\Omega(x_1, x_2, \dots, x_n))$, Lebesgue, with $\Omega(x_1, x_2, \dots, x_n)$ the phase space of n particles; such complex functions define a Hilbert-Koopman space \mathcal{H}_n .

An approach developed in terms of \mathcal{H}_n corresponds to a "first-quantized" representation of classical statistical mechanics and describes a system with a fixed number of particles, n . It is showed [26] that the functions $\theta_n = \theta(x_1, x_2, \dots, x_n; t) = \langle x_1, x_2, \dots, x_n | \theta_n(t) \rangle$, ($|\theta_n(t)\rangle \in \mathcal{H}_n$) satisfy the equation

$$\begin{aligned} \partial_t \theta_n &= \{h_n, \theta_n\}_n \\ &= -iL_n \theta_n; \quad L_n = i\{h_n, \}_n. \end{aligned} \tag{8}$$

Hence, if we define $f(x_1, x_2, \dots, x_n; t) = |\theta(x_1, x_2, \dots, x_n; t)|^2$, we obtain a solution of the Liouville equation, since the square of the absolute value of any solution of Eq.(8) is solution of Eq.(1). A consistent physical interpretation is gotten since $|\theta_n|^2$ is interpreted as the distribution function of n -particles in phase space. It follows that $|\chi_n\rangle$ describes a n -particle state for which the particles are at points $x_i = (q_i, p_i)$, $i = 1, 2, \dots, n$ of $\Omega(x_1, x_2, \dots, x_n)$, and $|\chi(t)\rangle$ is a classical nonstationary grand-ensemble state.

In this “second-quantized” formalism, a physical quantity, corresponding to a n -point dynamical variable, is represented by a linear Hermitian operator as

$$A = \frac{1}{n!} \int \psi^*(x_1; t) \psi^*(x_2; t) \dots \psi^*(x_n; t) a(x_1, x_2, \dots, x_n) \psi(x_1; t) \psi(x_2; t) \dots \psi(x_n; t) d^n x, \quad (9)$$

where $a(x_1, x_2, \dots, x_n)$ is a “first-quantized” operator defined on \mathcal{H}_n . The possible numerical values of a classical quantity described by A are its eigenvalues, and the average value is given by

$$\langle A \rangle = \langle \chi(t) | A | \chi(t) \rangle.$$

As in quantum theory, three pictures can be introduced for both the state vector $|\chi(t)\rangle$ and the operator of this formalism, namely, a classical Schrödinger picture, a classical Heisenberg picture and a classical interaction picture. In the former, the operators are considered as time-independent whilst the functional state $|\chi(t)\rangle$ is time dependent. Then, we have $|\chi_S(t)\rangle = U(t, t_o) |\chi(t_o)\rangle$, with $U(t_o, t_o) = 1$ and

$$U(t, t_o) = \exp[-i(t - t_o)L],$$

if L does not depend on time explicitly. The classical Heisenberg picture is defined by the transformation (the indexes (H) refers to the classical Schrödinger (Heisenberg) picture)

$$\begin{aligned} |\chi_H(t)\rangle &= \exp(itL) |\chi_S(t)\rangle, \\ A_H(t) &= \exp(itL) A_S(t) \exp(-itL). \end{aligned}$$

For this picture, it follows that

$$\begin{aligned} \partial_t |\chi_H(t)\rangle &= 0, \\ i\partial_t A_H &= [A_H, L], \end{aligned} \quad (10)$$

while Eq.(5) refers to the classical Schrödinger picture.

In the classical Heisenberg picture the field operator obeys the motion equation

$$\begin{aligned} \partial_t \psi(x, t) &= -\frac{p}{m} \frac{\partial}{\partial q} \psi(x; t) + \int dx' \psi^*(x', t) \left\{ \frac{\partial V(q, q')}{\partial q} \frac{\partial}{\partial p} \right. \\ &\quad \left. + \frac{\partial V(q, q')}{\partial q'} \frac{\partial}{\partial p'} \right\} \psi(x'; t) \psi(x; t), \end{aligned}$$

and the density of probability of n -body in the phase space, $f(x_1, x_2, \dots, x_n; t)$, is defined thus

$$\begin{aligned} f(x_1, x_2, \dots, x_n; t) &= \langle \chi_n | \psi^*(x_1; t) \psi^*(x_2; t) \dots \psi^*(x_n; t) \\ &\quad \times \psi(x_1; t) \psi(x_2; t) \dots \psi(x_n; t) | \chi_n \rangle. \end{aligned}$$

Ending this section, we would like to emphasize that the classical statistical mechanics developed in this scenario of vector (Fock) space, analogue to the quantum field theory, presents, beyond elegance, some formal and practical advantages. In particular, there exists a double structure revealed in the nature of the operators. Indeed, we notice that the generator of time evolution, the Liouvillian, is different from the Hamiltonian of the system. Such a doubling, in algebraic terms, is the same as that one arising in quantum thermofield-dynamics formalism[43]. This aspect will be set up in a more evident way in the next section, where we will explore

some aspects of symmetry in this phase space field theory. The conservation laws, a central point to build a nonequilibrium statistical operator, will be then written in a local form.

III. Aspects of symmetry and local conservation laws

First of all, let us write down the expressions of the main important operators for the development of this work, using the definition given by Eq.(9). They are (as longer as there is no confusion, hereafter we adopt the summation convention for repeated indices):

Generator of time translations (the Liouvillian, Eq.(6)),

$$\begin{aligned}
 L &= -i \int dx L(x,t), \\
 L(x,t) &= \psi^*(x;t) \frac{p}{m} \frac{\partial}{\partial q} \psi(x;t) \\
 &\quad - \frac{1}{2} \int dx dx' \psi^*(x;t) \psi^*(x';t) \left(\frac{\partial V(q,q')}{\partial q} \frac{\partial}{\partial p} \right. \\
 &\quad \left. + \frac{\partial V(q,q')}{\partial q'} \frac{\partial}{\partial p'} \right) \psi(x';t) \psi(x;t),
 \end{aligned}
 \tag{11}$$

Generator of phase space translations,

$$\begin{aligned}
 \Pi_a &= -i \int dx \Pi_a(x;t), \\
 \Pi_a(x;t) &= \psi^*(x;t) \left(\frac{\partial}{\partial q_a} + \frac{\partial}{\partial p_a} \right) \psi(x;t), \quad a = 1, 2, 3.
 \end{aligned}
 \tag{12}$$

Generator of phase space rotations,

$$\begin{aligned}
 M_a &= i \varepsilon_{abc} \int dx M_{bc}(x;t), \quad a, b, c = 1, 2, 3 \\
 M_{bc}(x;t) &= \psi^*(x;t) \left(q_c \frac{\partial}{\partial q_b} + p_c \frac{\partial}{\partial p_b} \right) \psi(x;t),
 \end{aligned}
 \tag{13}$$

Hamiltonian operator,

$$\begin{aligned}
 h &= \int dx h(x;t), \\
 h(x;t) &= \psi^*(x;t) \frac{p^2}{2m} \psi(x;t) \\
 &\quad + \frac{1}{2} \int dx dx' \psi^*(x;t) \psi^*(x';t) V(q,q') \psi(x;t) \psi(x';t),
 \end{aligned}
 \tag{14}$$

Linear momentum operator,

$$\begin{aligned}
 \pi_a &= \int dx \pi_a(x;t), \\
 \pi_a(x;t) &= p_a \psi^*(x;t) \psi(x;t),
 \end{aligned}
 \tag{15}$$

Angular momentum operator

$$\begin{aligned} \mathbf{m}_a &= i\varepsilon_{abc} \int dx \mathbf{m}_{bc}(x;t) , \\ \mathbf{m}_{bc}(x;t) &= \psi^*(x;t) q_b p_c \psi(x;t). \end{aligned} \quad (16)$$

If we define the operators

$$\mathbf{B}_a = i \int dx \psi^*(x;t) \left(t \frac{\partial}{\partial q_a} + im \frac{\partial}{\partial p_a} \right) \psi(x;t), \quad (17)$$

and

$$\mathbf{b}_a = i \int dx \psi^*(x;t) (mq_a - tp_a) \psi(x;t) \quad (18)$$

a representation for the Lie algebra of the Galilei group can be derived. That is, the generator of the symmetries in this representation, Eqs.(11)–(17), satisfy

$$[\mathbf{M}_a, \mathbf{M}_b] = i\varepsilon_{abc} \mathbf{M}_c, \quad (19)$$

$$[\mathbf{M}_a, \mathbf{\Pi}_b] = i\varepsilon_{abc} \mathbf{\Pi}_c, \quad (20)$$

$$[\mathbf{M}_a, \mathbf{B}_b] = i\varepsilon_{abc} \mathbf{B}_c, \quad (21)$$

$$[\mathbf{B}_a, \mathbf{L}] = i\mathbf{\Pi}_a, \quad (22)$$

$$[\mathbf{B}_a, \mathbf{\Pi}_b] = 0. \quad (23)$$

\mathbf{B} plays the role of Galilei boost. There are ancillary commutation relations, showing how the observables are transformed under the Galilei generators; for instance, for the observable operators \mathbf{h} , $\mathbf{\pi}$, \mathbf{m} and \mathbf{b} , we have

$$[\mathbf{M}_a, \mathbf{m}_b] = i\varepsilon_{abc} \mathbf{m}_c, \quad (24)$$

$$[\mathbf{M}_a, \mathbf{\pi}_b] = i\varepsilon_{abc} \mathbf{\pi}_c, \quad (25)$$

$$[\mathbf{B}_a, \mathbf{h}] = i\mathbf{\pi}_a, \quad (26)$$

$$[\mathbf{B}_a, \mathbf{\pi}_b] = im\delta_{ab}, \quad (27)$$

$$[\mathbf{\Pi}_a, \mathbf{b}_b] = im\delta_{ab}. \quad (28)$$

So the operators \mathbf{b}/m can be interpreted as the position operator of the theory, whilst m is the mass.

We notice that to each generator of symmetry there is an associated observable, both described by different elements of the Lie algebra given by Eqs.(19)–(28). This is a thermofield-dynamics Lie algebra[23, 43], and so, the Schönberg's approach is its classical representation.

The invariants of this formalism can be derived from Eq.(10), via the condition

$$[\mathbf{A}, \mathbf{L}] = 0. \quad (29)$$

Then requiring the hypothesis of isotropy and homogeneity of the space-time and the condition (29), we can show that there exists seven basic invariants in this formalism: the six operators given by Eqs.(11)–(16) plus the conservation of mass, which can be expressed by the fact that $[\mathbf{L}, \mathbf{n}] = 0$, where \mathbf{n} , the number operator, is given by Eq.(7)

$$\mathbf{n} = \int dx \mathbf{n}(x;t); \quad \mathbf{n}(x;t) = \psi^*(x;t)\psi(x;t). \quad (30)$$

In order to build the nonequilibrium statistical operator, we obtain from Eq. (29), with \mathbf{A} standing for each of the operators $\mathbf{L}, \mathbf{\Pi}, \mathbf{M}, \mathbf{h}, \mathbf{\pi}, \mathbf{m}$, and \mathbf{n} , the conservation laws in a local form, using Eqs.(11)–(16) and (30). First, to set the notation, we define

$$\mathbf{p} = (p_1, p_2, p_3), \quad \mathbf{q} = (q_1, q_2, q_3)$$

$$\begin{aligned} \nabla_x &= \left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p} \right) \text{ with} \\ \frac{\partial}{\partial q} &= \nabla_q = \left(\frac{\partial}{\partial q_1}, \frac{\partial}{\partial q_2}, \frac{\partial}{\partial q_3} \right), \\ \frac{\partial}{\partial p} &= \nabla_p = \left(\frac{\partial}{\partial p_1}, \frac{\partial}{\partial p_2}, \frac{\partial}{\partial p_3} \right), \\ V(q, q') &= V(|q - q'|), \\ \sum_{a=1}^3 \frac{\partial}{\partial x_a} &= \left(\sum_{a=1}^3 \frac{\partial}{\partial q_a}, \sum_{a=1}^3 \frac{\partial}{\partial p_a} \right) \end{aligned}$$

and the currents $J_m(x; t)$ are defined by

$$J_m(x; t) = (J_{m,q}(x; t), J_{m,p}(x; t)), \quad m = 0, 1, 2, \dots, 6, \tag{31}$$

with $\nabla_x \cdot J_m(x; t) = \nabla_q \cdot J_{m,q}(x; t) + \nabla_p \cdot J_{m,p}(x; t)$. Then, we have the following continuity equation for the densities $L(x; t)$, $\Pi(x; t)$, $M(x; t)$, $h(x; t)$, $\pi(x; t)$, $m(x; t)$, and $n(x; t)$:

Generator of time translation, $L(x; t)$,

$$\partial_t L(x; t) + \nabla_x \cdot J_o(x; t) = 0 \quad , \tag{32}$$

where

$$\begin{aligned} J_{o,q}(x; t) &= -\frac{3i}{2m} \int \nabla_q V(q, q') \psi^*(x; t) \psi^*(x'; t) \psi(x'; t) \psi(x; t) dx' \\ &\quad -i \frac{p}{m} \left\{ \frac{p}{m} \cdot \nabla_q (\psi^*(x; t) \psi(x; t)) \right. \\ &\quad - \int [\nabla_q V(q, q') \psi^*(x'; t) \psi^*(x; t) \cdot \nabla_p \psi(x; t) \psi(x'; t) \\ &\quad \left. + \nabla_{q'} V(q, q') \psi^*(x; t) \psi^*(x'; t) \cdot \nabla_{p'} \psi(x'; t) \psi(x; t)] dx' \right\} \\ &\quad - \frac{i}{4} \int (q - q') \nabla_q \cdot (\nabla_{q'} V(q, q')) F(x, x') dx', \end{aligned}$$

with

$$\begin{aligned} F(x, x') &= \psi^*(x'; t) \frac{p}{m} \cdot (\nabla_p \psi^*(x; t) \psi(x; t)) \psi(x'; t) \\ &\quad - \psi^*(x; t) \frac{p}{m} \cdot (\nabla_{p'} \psi^*(x'; t) \psi(x'; t)) \psi(x; t) \\ &\quad + \psi^*(x; t) \psi^*(x'; t) \frac{p'}{m} \cdot \nabla_{p'} \psi(x'; t) \psi(x; t) \\ &\quad - \psi^*(x'; t) \psi^*(x; t) \frac{p'}{m} \cdot \nabla_p \psi(x; t) \psi(x'; t) \\ &\quad + \frac{3}{m} \psi^*(x; t) \psi^*(x'; t) \psi(x'; t) \psi(x; t), \end{aligned}$$

and

$$\begin{aligned} J_{o,p}(x; t) &= \frac{i}{2} \int \left\{ \nabla_q V(q, q') \frac{p}{m} \cdot \nabla_q (\psi^*(x; t) \psi^*(x'; t) \psi(x'; t) \psi(x; t)) \right. \\ &\quad - \nabla_q V(q, q') \psi^*(x'; t) \\ &\quad \left(\int \nabla_q V(q, q'') \psi^*(x''; t) \psi^*(x; t) \cdot \nabla_p \psi(x; t) \psi(x''; t) dx'' \right) \psi(x'; t) \\ &\quad - \nabla_{q'} V(q, q') \psi^*(x'; t) \psi^*(x; t) \\ &\quad \left. \left(\int \psi^*(x''; t) \nabla_{q''} \psi(x''; t) dx'' \right) \psi(x; t) \cdot \nabla_{p'} \psi(x'; t) \right\} dx'. \end{aligned}$$

Generator of translation in phase space, $\Pi(x)$,

$$\partial_t \Pi(x; t) + \nabla_x \cdot J_1(x; t) = 0, \quad (33)$$

with

$$J_{1,q}(x; t) = \psi^*(x; t) \frac{p}{m} \sum_{a=1}^3 \left(\frac{\partial}{\partial q_a} + \frac{\partial}{\partial p_a} \right) \psi(x; t),$$

and

$$J_{1,p}(x; t) = -\psi^*(x; t) \int \psi^*(x'; t) \frac{\partial V(q, q')}{\partial q} \psi(x'; t) dx' \sum_{a=1}^3 \left(\frac{\partial}{\partial q_a} + \frac{\partial}{\partial p_a} \right) \psi(x; t).$$

Generator of rotations in phase space, $M(x)$,

$$\partial_t M(x; t) + \nabla_x \cdot J_2(x; t) = 0, \quad (34)$$

with

$$J_{2,q}(x; t) = \psi^*(x; t) \frac{p}{m} \sum_{a=1}^3 \varepsilon_{abc} (q_b \frac{\partial}{\partial q_c} + p_b \frac{\partial}{\partial p_c}) \psi(x; t),$$

and

$$J_{2,p}(x; t) = -\psi^*(x; t) \left(\int \psi^*(x'; t) \frac{\partial V(q, q')}{\partial q} \psi(x'; t) dx' \right) \times \sum_{a=1}^3 \varepsilon_{abc} \left(q_a \frac{\partial}{\partial q_b} + p_a \frac{\partial}{\partial p_b} \right) \psi(x; t).$$

Hamiltonian, $h(x; t)$,

$$\partial_t h(x; t) + \nabla_x \cdot J_3(x; t) = 0, \quad (35)$$

$$J_{3,q}(x; t) = \frac{p}{m} \psi^*(x; t) \frac{p^2}{2m} \psi(x; t) + \frac{1}{2} \int V(q, q') \psi^*(x'; t) \psi^*(x; t) \frac{p}{m} \psi(x; t) \psi(x'; t) dx' - \frac{1}{4} \int (q - q') \nabla_q V(q, q') \cdot (\psi^*(x'; t) \psi^*(x; t) \frac{p}{m} \psi(x; t) \psi(x'; t) + \psi^*(x; t) \psi^*(x'; t) \frac{p'}{m} \psi(x'; t) \psi(x; t)) dx'$$

$$J_{3,p}(x; t) = -\frac{p^2}{2m} \psi^*(x; t) \int \psi^*(x'; t) \nabla_q V(q, q') \psi(x'; t) dx' \psi(x; t) - \frac{1}{2} \int V(q, q') \psi^*(x'; t) \psi^*(x; t) \left(\int \psi^*(x''; t) \nabla_q V(q, q'') \psi(x''; t) dx'' \right) \psi(x; t) \psi(x'; t) dx'.$$

Linear momentum, $\pi_b(x; t)$, $b = 1, 2, 3$,

$$\partial_t \pi_b(x; t) + \nabla_x \cdot J_4(x; t) = 0, \quad (36)$$

$$\text{with } \nabla_x \cdot J_4(x; t) = \sum_{a=1}^3 \frac{\partial}{\partial x_a} T_{ab}(x; t)$$

where $T_{ab}(x;t) = (T_{ab}^{(q)}(x;t), T_{ab}^{(p)}(x;t))$, with

$$T_{ab}^{(q)}(x;t) = \frac{p_a}{m} \psi^*(x;t) p_b \psi(x;t) - \frac{1}{2} \int (q_a - q'_a)(q_b - q'_b) \frac{1}{r} \frac{dV(r)}{dr} \cdot \psi^*(x;t) \psi^*(x';t) \psi(x';t) \psi(x;t) dx', \tag{37}$$

$r = |q - q'|$ and

$$T_{ab}^{(p)}(x;t) = -p_b \psi^*(x;t) \int \psi^*(x';t) \frac{\partial V(q, q')}{\partial q_a} \psi(x';t) dx' \psi(x;t). \tag{38}$$

Angular momentum density, $m_{ab}(x)$, $a, b = 1, 2, 3$

$$\partial_t m_{ab}(x;t) + \nabla_x \cdot J_5(x;t) = 0, \tag{39}$$

with

$$\nabla_x \cdot J_5(x;t) = \sum_{c=1}^3 \frac{\partial}{\partial x_c} (q_a T_{cb}(x;t) - q_b T_{ca}(x;t))$$

where

$$m_{ab}(x;t) = \psi^*(x;t) q_a p_b \psi(x;t) - \psi^*(x;t) q_b p_a \psi(x;t),$$

and $T_{ab}(x;t) = (T_{ab}^{(q)}(x;t), T_{ab}^{(p)}(x;t))$ is given by Eqs.(37) and (38).

Particle number, $n(x;t)$,

$$\partial_t n(x;t) + \nabla_x \cdot J_6(x;t) = 0, \tag{40}$$

where $J_6(x;t) = (J_{6,q}(x;t), J_{6,p}(x;t))$, with

$$J_{6,q}(x;t) = \psi^*(x;t) \frac{p}{m} \psi(x;t),$$

and

$$J_{6,p}(x;t) = -\psi^*(x;t) \int \psi^*(x';t) \frac{\partial V(q, q')}{\partial q} \psi(x';t) dx' \psi(x;t).$$

In short, we write these equations as

$$\partial_t \alpha_m(x;t) + \nabla_x \cdot J_m(x;t) = 0, \quad m = 0, 1, 2, \dots, 6, \tag{41}$$

where

$$\begin{aligned} \alpha_0(x;t) &= L(x;t), & \alpha_1(x;t) &= \Pi(x;t), & \alpha_2(x;t) &= M(x;t), \\ \alpha_3(x;t) &= h(x;t), & \alpha_4(x;t) &= \pi(x;t), & \alpha_5(x;t) &= m(x;t), \\ \alpha_6(x;t) &= n(x;t). \end{aligned}$$

Comparing our local conservation laws with those derived in the context of quantum statistical mechanics, we note that the currents $J_m(x;t)$ depend not only on q , as in the quantum case, but also on p . Moreover, it should be interesting to point out that in order to determine such (phase space) conservation laws, we have used the correspondent hypothesis employed in the derivation of NSO in quantum case (for instance,

given an operator $O(x)$, $x = (q, p)$, we are interested in integrals of type $\int F(x)O(x) dx$, where $F(x)$ is some arbitrary vector function of the phase space coordinates, that varies little over distances of order in the range of interaction forces between particles). Such a development has been so possible because this phase space field theory is based on a mathematical structure similar to

that of quantum theory.

With such conservation laws written in a local form, we can build an expression of the NSO in this classical thermofield dynamics formalism. This is the subject of next section where, as an application, we consider a gas in contact with a thermostat to derive the Fokker-Planck-Kramers equation.

IV. Nonequilibrium statistical operator and Fokker-Planck-Kramers equation

As it is usual to derive the NSO operator, we assume that the state of a nonequilibrium system, for short interval of time, depends on a finite set of macroscopic parameters, which are, in turn, analytic functions of

space position and time. We are looking for an operator $\rho(t)$ which obeys the Liouville equation in its “second quantized” version, Eq.(10), that is

$$i\partial_t\rho(t) = [\rho(t), L]. \quad (42)$$

At this point, one advantage of using the second quantized version of the classical statistical mechanics arises associated with its vector structure. In fact, we note that Eq.(42) is, in form, identical to the quantum case, except, as we are dealing with a classical system, that the generator of temporal evolution is the second quantized Liouvillian L (not a Hamiltonian) given in Eq.(6). In spite of this fact, however, we can follow, from Eq.(42), step-by-step, the quantum case (which can be found, for instance, in refs.[1, 12]). The differences from the quantum situation will emerge when the NSO operator is explicitly written. Then, the final result is given by (in this section, we consider all the operators in the classical Heisenberg picture)

$$\begin{aligned} \rho(t) = & \exp\{-\Phi(t) - \sum_m \int [\alpha_m(x)a_m(x;t) - \int_{-\infty}^{\circ} e^{\epsilon t_1}(\nabla_x a_m(x;t+t_1) \cdot \\ & \cdot J_m(x;t_1) + \frac{\partial a_m(x;t+t_1)}{\partial t_1} \alpha_m(x;t+t_1))dt_1]dx\}, \end{aligned} \quad (43)$$

where

$$\begin{aligned} \Phi(t) = & \ln Tr\{\exp[-\int \sum_m \alpha_m(x)a_m(x;t) - \int_{-\infty}^{\circ} e^{\epsilon t_1}(\dot{a}_m(x;t_1) \cdot \\ & a_m(x;t+t_1) + \dot{\alpha}_m(x;t_1)a_m(x;t+t_1))dt_1]dt\} \end{aligned}$$

is the Massieu-Planck functional. The parameters $a_m(x;t)$ are the intensive thermodynamical variables conjugated to the extensive variables $A_m(t)$, defined by $A_m(t) = \langle \alpha_m \rangle_t^t = Tr[\alpha_m \rho]$. The quantities α_m and J_m ($m = 0, 1, 2, \dots, 6$) are the densities and the corresponding fluxes given in the previous Section. Eq.(43) gives the NSO in classical thermofield dynamics in its general form. If we are interested in some specific system we choose the convenient α_m and J_m to compose $\rho(t)$.

Let us apply this method to derive the Fokker-Planck-Kramers equation. We consider s subsystems in contact to a thermostat (which is in thermal equilibrium), and the subsystems are supposed not to interact

to each other. In this situation, the “second quantized” Liouvillian can be written as

$$L = L_o + L_{ther} + L_{in},$$

where L_o , the Liouvillian of the subsystems, is defined by

$$L_o = i \int dx \psi^*(x;t) \left(\frac{\partial h_o}{\partial q} \frac{\partial}{\partial p} - \frac{\partial h_o}{\partial p} \frac{\partial}{\partial q} \right) \psi(x;t);$$

L_{ther} is the Liouvillian for the thermostat, with phase space variables $X = (Q, P)$; and L_{in} is the interaction Liouvillian between the subsystems and thermostat, specified here by

$$L_{in} = i \int \int dx dX \psi^*(X;t)\psi^*(x;t) \left(\frac{\partial h_{in}}{\partial q} \frac{\partial}{\partial p} - \frac{\partial h_{in}}{\partial p} \frac{\partial}{\partial q} \right) \psi(x;t)\psi(X;t).$$

$h_o = h_o(x)$ is the Hamiltonian for a generic subsystem, and $h_{in} = h_{in}(x, X)$ is the interaction Hamiltonian between the generic subsystem and the thermostat.

The macroscopic state of the system is assumed to be fully characterized by the function $f(x, t)$ defined by

$$f(x, t) = Tr[\rho(t)n(t)], \tag{44}$$

where $n(t)$ is the density number operator and $\rho(t)$ is the NSO. Assuming the conservation of mass, we can write the equation for $n(t)$ as a continuity equation, given by Eq.(40), that now takes the form

$$\dot{n}(x; t) + \nabla_x \cdot J_6(x) = 0; \tag{45}$$

$J_6(x) = (J_{6q}(x), J_{6p}(x))$, the flow density, is specified by

$$\begin{aligned} J_{6q}(x) &= \frac{\partial h_o(x)}{\partial p} + \frac{\partial h_{in}(x, X)}{\partial p}, \\ J_{6p}(x) &= \frac{\partial h_o(x)}{\partial q} + \frac{\partial h_{in}(x, X)}{\partial q}, \end{aligned}$$

where we are using the notation

$$\begin{aligned} \frac{\partial h_o(x)}{\partial p} &= \psi^*(x;t) \frac{\partial h_o}{\partial p} \psi(x;t), \\ \frac{\partial h_o(x)}{\partial q} &= -\psi^*(x;t) \frac{\partial h_o}{\partial q} \psi(x;t), \\ \frac{\partial h_{in}(x, X)}{\partial p} &= \int dX \psi^*(X;t)\psi^*(x;t) \frac{\partial h_{in}}{\partial p} \psi(x;t)\psi(X;t) \\ \frac{\partial h_{in}(x, X)}{\partial q} &= -\int dX \psi^*(X;t)\psi^*(x;t) \frac{\partial h_{in}}{\partial q} \psi(x;t)\psi(X;t). \end{aligned}$$

Using the conservation law Eq.(45) with the energy flow equation, we write Eq.(43) explicitly, picking up as the non-null variables $\alpha_3(x;t) = h(t)$, with the corresponding thermal variable $a_3(x;t) = \beta(x;t)$, and $\alpha_6(x;t) = n(x;t)$, with $a_6(x;t) = -\beta(x;t)\varphi(x;t)$, resulting then in

$$\begin{aligned} \rho(t) &= \exp\{-\Phi(t) - \int [\beta(x;t)h(x;t) - \beta(x;t)\varphi(x;t)n(x;t) \\ &+ \beta(x) \int_{-\infty}^o e^{\epsilon t_1} \left(\frac{\partial \varphi(x;t+t_1)}{\partial q} J_{6q}(x) + \frac{\partial \varphi(x;t+t_1)}{\partial p} J_{6p}(x) \right) \\ &+ \dot{\varphi}(x;t+t_1)n(x;t)] dt_1] dx\}. \end{aligned} \tag{46}$$

The function $\varphi(x;t)$ can be determined assuming the condition

$$\langle n(x;t) \rangle = \langle n(x;t) \rangle_{loc}. \tag{47}$$

Here $\langle \dots \rangle$ is indicating the average with $\rho(t)$, and $\langle \dots \rangle_{loc}$ is an average under the local statistical operator, defined from $\rho(t)$ by discarding the flow terms, that is

$$\rho(t) = \exp\{-\bar{\Phi}(t) - \int [\beta(x;t)h(x;t) - \beta(x;t)\varphi(x;t)n(x;t)] dx\};$$

$\bar{\Phi}(t)$ is the Massieu-Planck functional for the local situation.

Eq.(46) under condition (47) corresponds, in the classical thermofield dynamics, to the result derived by Zubarev [1] in the (usual) classical statistical mechanics. Then, from this point, we can follow according to Zubarev to derive an equation for $f(x, t)$, where $f(x, t)$ is defined in Eq.(44). In this way we get

$$\begin{aligned}
 & \dot{f}(x, t) + \left(\frac{\partial h_o(x)}{\partial p} + \frac{\langle h_{in}(x, X) \rangle_o}{\partial p} \right) \frac{\partial f}{\partial q} \\
 & - \left(\frac{\partial h_o(x)}{\partial q} + \frac{\langle h_{in}(x, X) \rangle_o}{\partial q} \right) \frac{\partial f}{\partial p} \\
 = & \frac{\partial}{\partial q} \left[L_{11}(x) \left(\frac{\partial h_o(x)}{\partial q} f(x; t) + k_B T \frac{\partial f(x; t)}{\partial q} \right) \right. \\
 & \left. - L_{12}(x) \left(\frac{\partial h_o(x)}{\partial p} f(x; t) + k_B T \frac{\partial f(x; t)}{\partial p} \right) \right] \\
 & - \frac{\partial}{\partial p} \left[L_{21}(x) \left(\frac{\partial h_o(x)}{\partial q} f(x; t) + k_B T \frac{\partial f(x; t)}{\partial q} \right) \right. \\
 & \left. - L_{22}(x) \left(\frac{\partial h_o(x)}{\partial p} f(x; t) + k_B T \frac{\partial f(x; t)}{\partial p} \right) \right], \tag{48}
 \end{aligned}$$

where $\langle \cdot \cdot \rangle_o$ means an canonical equilibrium average, k_B the Boltzmann constant and T the temperature of the thermostat. The kinetic coefficients L_{11} , L_{12} , L_{21} , and L_{22} are given by

$$\begin{aligned}
 L_{11}(x) &= \frac{1}{k_B T} \int_{-\infty}^0 dt e^{\epsilon t} \left\langle \frac{\partial h_{in}(x, X)}{\partial p} \frac{\partial h_{in}(x, X; t)}{\partial p} \right\rangle_o, \\
 L_{12}(x) &= \frac{1}{k_B T} \int_{-\infty}^0 dt e^{\epsilon t} \left\langle \frac{\partial h_{in}(x, X)}{\partial p} \frac{\partial h_{in}(x, X; t)}{\partial q} \right\rangle_o, \\
 L_{21}(x) &= \frac{1}{k_B T} \int_{-\infty}^0 dt e^{\epsilon t} \left\langle \frac{\partial h_{in}(x, X)}{\partial q} \frac{\partial h_{in}(x, X; t)}{\partial p} \right\rangle_o, \\
 L_{22}(x) &= \frac{1}{k_B T} \int_{-\infty}^0 dt e^{\epsilon t} \left\langle \frac{\partial h_{in}(x, X)}{\partial q} \frac{\partial h_{in}(x, X; t)}{\partial q} \right\rangle_o.
 \end{aligned}$$

Eq.(48) is the Fokker-Planck-Kramers equation, written in the Schönberg phase-space field formalism, describing the behavior of subsystems in contact with a thermostat.

V. Final remarks and conclusions

In this paper we have proposed a nonequilibrium statistical operator (NSO), to describe classical systems, based on a phase space field theory, using methods of the number representation first developed for quantum field theory. Then, in this approach, the field operators, $\psi(x)$, $x = (q, p)$, which are introduced in a second quantized version in the classical phase space, hold a representation for the Galilei group, associated with the algebraic structure of the thermofield dynamics formalism. Indeed, the field operators in phase-space, written in terms of $\psi(x)$, present a double structure, which can be considered as a representation of

w*-algebras from which the Lie algebra of thermal field theories emerge [23].

From the analysis of symmetries, we have presented the constants of motion in terms of the field operators and the equations of conservation have been written in a local form. This is a relevant feature of our work, which allows the introduction of a classical NSO on new grounds. This method has been used to derive the Fokker-Planck-Kramers equation, and doing so, we have shown as this classical NSO works in a specific example. Beyond that, we could analyse our procedure in comparison with standard methods.

We would like to emphasize that the method of second-quantized operators in phase space, used here in a non relativistic classical problem, can be generalized for relativistic situations. This is a work to appear elsewhere.

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