

Classical stochastic approach to quantum mechanics and quantum thermodynamics

Mário J. de Oliveira

Universidade de São Paulo, Instituto de Física, Rua do Matão, 1371, 05508-090 São Paulo, SP, Brazil

We derive the equations of quantum mechanics and quantum thermodynamics from the assumption that a quantum system can be described by an underlying classical system of particles. Each component ϕ_j of the wave vector is understood as a stochastic complex variable whose real and imaginary parts are proportional to the coordinate and momentum associated to a degree of freedom of the underlying classical system. From the classical stochastic equations of motion, we derive a general equation for the covariance matrix of the wave vector which turns out to be of the Lindblad type. When the noise changes only the phase of ϕ_j , the Schrödinger and the quantum Liouville equation are obtained. The component ψ_j of the wave vector obeying the Schrödinger equation is related to stochastic wave vector by $|\psi_j|^2 = \langle |\phi_j|^2 \rangle$.

I. INTRODUCTION

A distinguishing feature of quantum mechanics [1–8] is its formulation in terms of an unobservable: the wave function. The presence of unobservables in a theory does not make it unscientific, as long as they lead to observables, that is, to quantities that can be observed or measured experimentally [9]. Any scientific theory has unobservables to a greater or lesser extent. Significant examples are the epicycles of Ptolemy, the aether of Newton, and the luminiferous aether of Maxwell. Much less obvious examples are the concepts of time reversibility, causality, homogeneity of time and homogeneity of space. The unobservable of quantum mechanics was present in its very beginning when Schrödinger formulated his equation in terms of the wave function. Although the wave function is an *unobservable* it leads through this equation to the *observable* spectral lines of hydrogen.

The question that we address here concerns the possibility of the formulation of quantum mechanics an unobservable other than the wave function. Specifically, the unobservable that we consider here to describe a quantum system is a system of particles obeying the classical equations of motion [10–13], which we call the *underlying* system to avoid confusion with a real system described by classical mechanics.

The standard formulation of quantum mechanics postulates that the quantum states are represented by wave vectors belonging to a complex vector space, the Hilbert space. In contrast, classical mechanics is represented in the Hamilton formulation by canonical variables belonging to a real vector space, the phase space. Thus a classical approach to quantum mechanics, requires a formulation of classical mechanics in terms of complex canonical variables.

The possibility of using complex variables to express the classical Hamilton equations of motion was pointed out by Lanczos [10] who showed that a pair of complex conjugate variables is also a pair of canonical variables. The formulation of the quantum equation of motion by a classical Hamilton equation in complex variables was given by Strocchi [14]. In his formulation a complex canonical variable is identified as a component ϕ_j , which

obeys the complex Hamilton equation associated to the Hamiltonian function \mathcal{H} , identified as the mean value

$$\mathcal{H} = \sum_j \phi_j^* H_{jk} \phi_k \quad (1)$$

of the Hamilton operator H .

An equivalent approach was proposed by Heslot [15] but instead of using a complex Hamilton equation, he shows that the real and imaginary parts of the wave functions are a pair of real classical canonical variables obeying the real standard Hamilton equation. The classical representation was then analyzed and explored by several authors [16–19].

A essential aspect of the classical representation concerns the norm of the wave vector,

$$\mathcal{N} = \sum_j \phi_j^* \phi_j, \quad (2)$$

which is a quantity conserved by the Hamilton equations of motion associated to the classical Hamiltonian (1). This is a nice property since according the wave vector should be normalized at all times. However, the conservation property does not determine the value of the norm. Therefore we should postulate that the norm has the same value for any possible trajectory in phase space as this is a basic postulate of quantum mechanics. More precisely, among all sectors of the phase space determined by distinct values of the norm, we must select just one of them. As we shall see, the one to be selected is connected to the Planck constant.

Quantum mechanics is understood as having a probabilistic character. However this character is not clearly manifested in the usual representation. For instance, no variable is considered to be a random variable. The probabilistic character is a consequence of the standard interpretation of quantum mechanics [20–22] which introduces probability in an ad-hoc and a posteriori manner by the proposition that the square of the absolute value of the wave function is a probability.

Here we introduce the probabilistic character in an explicit and a priori form by turning ϕ_j into a stochastic variable. This is accomplished by transforming the equation of motion into a stochastic equation through the

addition of a noise term in the Hamilton equations of motion [23–26]. The noise transforms the trajectories in the complex phase space into stochastic trajectories, and it is set up in such a way as to preserve the norm given by (2) along any stochastic trajectory.

The noise changes in general the absolute value and the phase of ϕ_k . A meaningful result of our analysis is that the Schrödinger and the quantum Liouville equations are obtained through noises that change the phase but not the absolute value of ϕ_k . This type of noise also makes each term of the norm constant. If the noise changes both the phase and the absolute value of ϕ_k then we reach the quantum thermodynamic equation which turns out to be the Lindblad equation for open system [27–30].

The quantum thermodynamic equation is the central equation of the quantum thermodynamics that we develop here. Based on this equation we derive the first law of thermodynamics and the second law of thermodynamics. This is accomplished by defining the quantum entropy and the quantum entropy production. The second law of thermodynamics is obtained by demonstrating that the entropy production is nonnegative. To demonstrate this proposition we use a reasoning similar to that employed by Spohn [31] which in turn was based on a theorem of Lieb [32].

II. STOCHASTIC EQUATION OF MOTION

A. Underlying classical system

The underlying system consists of a classical system with n degrees of freedom. Each degree of freedom corresponds to a pair of canonical variables q_i and p_i , and the Hamilton equations of motion are

$$\frac{dq_i}{dt} = \frac{\partial \mathcal{H}}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial q_i}, \quad (3)$$

which determine trajectories in the $2n$ dimensional phase space, which is the vector space spanned by the canonical variables. The Hamiltonian function is assumed to be of the form

$$\mathcal{H} = \frac{1}{2m} \sum_j p_j^2 + \frac{1}{2} \sum_{jk} K_{jk} q_j q_k, \quad (4)$$

which corresponds to a collection of n particles of mass m interacting harmonically. The coefficients K_{jk} are the entries of a $n \times n$ matrix K with positive eigenvalues. Using the notations q and p for the column matrices with elements q_j and p_j , respectively, we write

$$\mathcal{H} = \frac{1}{2m} p^\top p + \frac{1}{2} q^\top K q. \quad (5)$$

We perform a canonical transformation to write the Hamiltonian function in a more symmetric form in which it becomes invariant by the exchange of the coordinate

and momentum of a pair of canonically conjugate variables. Taking into account that K is Hermitian with nonnegative eigenvalues we may define the matrix $\Omega = K^{1/2}/\sqrt{m}$. It has nonnegative eigenvalues and is Hermitian. The canonical transformation $q \rightarrow x$ and $p \rightarrow y$ is defined by

$$x = (m\Omega)^{1/2} q \quad y = (m\Omega)^{-1/2} p, \quad (6)$$

and the Hamiltonian function becomes

$$\mathcal{H} = \frac{1}{2} y^\top \Omega y + \frac{1}{2} x^\top \Omega x,$$

and we see that \mathcal{H} is invariant by the exchange of x and y . In an explicit form,

$$\mathcal{H} = \frac{1}{2} \sum_{jk} \Omega_{jk} (x_j x_k + y_j y_k), \quad (7)$$

and the Hamilton equations of motion becomes

$$\frac{dx_i}{dt} = \frac{\partial \mathcal{H}}{\partial y_i}, \quad \frac{dy_i}{dt} = -\frac{\partial \mathcal{H}}{\partial x_i}. \quad (8)$$

Let us define the quantity

$$\mathcal{I} = \frac{1}{2} \sum_j (x_j^2 + y_j^2). \quad (9)$$

It follows from the Hamilton equations that \mathcal{I} is a constant of the motion, a property that allows us to divide the phase space in sectors, each one corresponding to a given value of \mathcal{I} . We then *postulate* that the only possible motions of the underlying system are those corresponding to a defined value \mathcal{I} . This value is denoted by μ ,

$$\frac{1}{2} \sum_j (x_j^2 + y_j^2) = \mu. \quad (10)$$

The constant μ has the physical dimension of (energy \times time) and it will be seen that μ is to be identified as the Planck constant. This postulate is the crucial step toward quantization within the present approach. It enables the appearance in the classical underlying system of the characteristic quantum properties such as the quantization of energy and the zero point of energy.

One can show that \mathcal{I} is an adiabatic invariant [33], that is, a slow change of the parameters of the Hamiltonian will change \mathcal{H} but not \mathcal{I} . This result connects the adiabatic invariance with quantization, an idea advanced by Ehrenfest which lead to the old quantum mechanics. The distinction between the approach of Ehrenfest from ours lies in his use of the invariant as connected to the motion of one quantum particle as if the particle itself was a classical particle.

In fact \mathcal{I} is not constant only in adiabatic changes but it is universally constant. Let us suppose that \mathcal{H} is time dependent, that is, Ω_{jk} depends on time. In this case \mathcal{H} is not a constant of motion because

$$\frac{d\mathcal{H}}{dt} = \frac{1}{2} \sum_{jk} \frac{d\Omega_{jk}}{dt} (x_j x_k + y_j y_k), \quad (11)$$

but

$$\frac{d\mathcal{I}}{dt} = 0 \quad (12)$$

This result allows to say that \mathcal{I} remains forever with the same value given at the initial time, even if \mathcal{H} is time dependent.

B. Classical dynamics in complex variables

The Hamilton equations of motion are written in terms of a set of $2n$ complex variables ϕ_j and ϕ_j^* , $j = 1, \dots, n$, obtained by the transformation

$$\phi_j = \frac{1}{\sqrt{2\mu}}(x_j + iy_j), \quad \phi_j^* = \frac{1}{\sqrt{2\mu}}(x_j - iy_j). \quad (13)$$

Using this transformation, we see that the expression (10) becomes

$$\sum_j \phi_j^* \phi_j = 1, \quad (14)$$

which expresses the postulate introduced above in terms of the complex variables.

The peculiar transformation from real to complex variables are canonical transformation leading to the following Hamilton equation of motion in complex variables

$$\frac{d\phi_j}{dt} = \frac{1}{i\mu} \frac{\partial \mathcal{H}}{\partial \phi_j^*}, \quad \frac{d\phi_j^*}{dt} = -\frac{1}{i\mu} \frac{\partial \mathcal{H}}{\partial \phi_j}, \quad (15)$$

where \mathcal{H} is the real bilinear function

$$\mathcal{H} = \sum_{jk} H_{jk} \phi_j^* \phi_k, \quad (16)$$

obtained from (7), where $H_{jk} = \mu(\Omega_{jk} + \Omega_{kj})/2$, and are the entries of a $n \times n$ Hermitian matrix H , that is, $H_{jk}^* = H_{kj}$, with positive eigenvalues. We remark that the complex variables ϕ_j and ϕ_j^* are dimensionless, which justifies the presence of the constant μ in the equations of motion.

The complex conjugate variables ϕ_j and ϕ_j^* are considered to be independent variables because their real and imaginary parts are proportional to the coordinate q_j and to the momentum p_j , which are independent. From the peculiar transformation above they also form a pair of canonically conjugate variables as is manifest in the equation of motion (15).

From the Hamilton equations of motion (15), the time evolution of a state function \mathcal{F} is

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\}, \quad (17)$$

where the term in the right-hand side is the Poisson brackets defined by

$$\{\mathcal{F}, \mathcal{H}\} = \sum_j \left(\frac{\partial \mathcal{F}}{\partial \phi_j} \frac{\partial \mathcal{H}}{\partial \phi_j^*} - \frac{\partial \mathcal{H}}{\partial \phi_j} \frac{\partial \mathcal{F}}{\partial \phi_j^*} \right), \quad (18)$$

If we replace \mathcal{F} by the norm of ϕ , defined by

$$\mathcal{N} = \sum_j \phi_j^* \phi_j, \quad (19)$$

we see that

$$\{\mathcal{N}, \mathcal{H}\} = 0, \quad (20)$$

which means that the norm is preserved along a trajectory in the complex vector space.

The value of \mathcal{N} cannot be arbitrary. In accordance with the postulate introduced above and expressed by equation (14), it should be equal to the unity. Using this result and writing the axes corresponding to a pair of canonical conjugate variables of the phase space as related to a complex variable ϕ_j , then the phase space becomes equivalent to a Hilbert space, which is a vector space with normalized vectors.

The form (16) of the Hamiltonian allows us to write the Hamilton equations in the form

$$\frac{d\phi_j}{dt} = \frac{1}{i\mu} \sum_k H_{jk} \phi_k. \quad (21)$$

Equivalently, we may write equation (21) in the vector form

$$i\mu \frac{d\phi}{dt} = H\phi. \quad (22)$$

If we set $\mu = \hbar$ and identify ϕ as the quantum state vector, we see that it is identical to the quantum equation that gives the time evolution of the state vector ϕ , or the Schrödinger equation.

C. Norm preserving noise

We now assume that ϕ follows a stochastic equation of motion which is the Hamilton equations supplemented by a noise term,

$$\frac{d\phi_j}{dt} = \frac{1}{i\mu} \sum_{jk} H_{jk} \phi_k + \zeta_j, \quad (23)$$

where ζ_j is a complex white noise, that is, its real and imaginary parts are white noises, and also depends on ϕ and ϕ^* . The noise will be set up in such a way that the norm \mathcal{N} is preserved along the stochastic trajectory in the complex vector space.

As it stands equation (23) has no precise meaning. To give it a precise meaning, we discretize the time in intervals τ and write the stochastic equation of motion in a discretized form. Let $\Delta\phi_j$ be the increment in ϕ_j when the time increases from t to $t + \tau$. Then the discretized version of equation (23) is assumed to be

$$\Delta\phi_j = \frac{\tau}{i\mu} \sum_k H_{jk} \phi_k + i\sqrt{\tau} \sum_k G_{jk} \phi_k - \frac{\tau}{2} \sum_k K_{jk} \phi_k, \quad (24)$$

where G_{jk} are independent random variables, which we consider to be the elements of a $n \times n$ matrix G , with zero mean, $\langle G_{jk} \rangle = 0$, and covariances

$$\langle G_{jk}^* G_{\ell m} \rangle = 2\gamma_{jk,\ell m}. \quad (25)$$

from which follows the property $\gamma_{jk,\ell m}^* = \gamma_{\ell m,jk}$. The quantities K_{jk} are related to G_{jk} and will be found by imposing the conservation of the norm. The elements G_{jk} and K_{jk} are understood as the entries of two $n \times n$ matrices G and K , respectively.

It is convenient to introduce a $n^2 \times n^2$ matrix Γ with elements Γ_{rs} which are related to $\gamma_{jk,\ell m}$. The index r has a one-to-one correspondence to (jk) and s has a one-to-one correspondence to (ℓm) . Using this convention, set $\Gamma_{rs} = \gamma_{r,s}$, or

$$\Gamma_{rs} = \langle G_r^* G_s \rangle. \quad (26)$$

From this relation it follows that Γ is a Hermitian matrix, $\Gamma_{rs}^* = \Gamma_{sr}$. Being Hermitian, Γ can be diagonalized by a unitary transformation. Denoting by Υ the $n^2 \times n^2$ matrix that diagonalizes Γ then $\Upsilon^\dagger \Gamma \Upsilon$ is diagonal and its elements λ_r are the eigenvalues of Γ . They are given by

$$\lambda_r = \sum_{s's} \Upsilon_{rs'}^\dagger \Gamma_{s's} \Upsilon_{sr}. \quad (27)$$

Using (26),

$$\lambda_r = \sum_{s's} \Upsilon_{rs'}^\dagger \langle G_{s'}^* G_s \rangle \Upsilon_{sr} = \langle |\sum_s G_s \Upsilon_{sr}|^2 \rangle, \quad (28)$$

and we see that $\lambda_r \geq 0$, that is the eigenvalues of the Hermitian matrix Γ are nonnegative, or in other words, Γ is a positive semi-definite matrix.

Let us determine the increment in the norm \mathcal{N} due to a change $\Delta\phi_j$ in the dynamic variables. It is given by

$$\Delta\mathcal{N} = \sum_j (\Delta\phi_j^* \phi_j + \phi_j^* \Delta\phi_j + \Delta\phi_j^* \Delta\phi_j). \quad (29)$$

Replacing $\Delta\phi_j$ in this equation, we find up to terms of order τ

$$\begin{aligned} \Delta\mathcal{N} &= i\sqrt{\tau} \sum_{jk} (G_{jk} - G_{kj}^*) \phi_j^* \phi_k \\ &\quad - \frac{\tau}{2} \sum_{jk} (K_{jk} + K_{kj}^*) \phi_j^* \phi_k + \tau \sum_{jk} (G^\dagger G)_{jk} \phi_j^* \phi_k. \end{aligned} \quad (30)$$

The terms containing H_{jk} vanish identically due to the Hermitian property $H_{jk}^* = H_{kj}$. Choosing

$$K = G^\dagger G, \quad (31)$$

which is the sought relation between K and G , and which we assume from now on, then the last two summations on the right-hand side of (30) vanish and

$$\Delta\mathcal{N} = i\sqrt{\tau} \sum_{jk} \phi_j^* (G - G^\dagger)_{jk} \phi_k. \quad (32)$$

If $G^\dagger = G$ then the increment vanishes and the norm \mathcal{N} is strictly constant along the stochastic trajectory. If this condition is not imposed, the increment in the norm will still vanish but in the average, that is, $\langle \Delta\mathcal{N} \rangle = 0$. The stochastic equation of motion (24) defines a Markovian stochastic dynamics which determines stochastic trajectories of ϕ in the vector space.

III. FUNDAMENTAL EQUATION

A. Probability density distribution

As the trajectories in the vector space are stochastic, we may ask for the probability of the occurrence of each trajectory. In the following we determine the equation that gives the time evolution of the probability density distribution $\mathcal{P}(\phi, \phi^*, t)$ of ϕ and ϕ^* at time t . We start by considering an arbitrary state function \mathcal{F} of ϕ and ϕ^* of the bilinear type

$$\mathcal{F} = \sum_{jk} F_{jk} \phi_j^* \phi_k, \quad (33)$$

where F_{jk} are understood as the complex entries of a $n \times n$ matrix F . The increment $\Delta\mathcal{F}$ of such a function is given by

$$\begin{aligned} \Delta\mathcal{F} &= \sum_j \frac{\partial\mathcal{F}}{\partial\phi_j} \Delta\phi_j + \sum_j \frac{\partial\mathcal{F}}{\partial\phi_j^*} \Delta\phi_j^* \\ &\quad + \sum_{jk} \frac{\partial^2\mathcal{F}}{\partial\phi_j \partial\phi_k^*} \Delta\phi_j \Delta\phi_k^*. \end{aligned} \quad (34)$$

Replacing $\Delta\phi_j$ in this equation we find up to terms of order τ

$$\begin{aligned} \Delta\mathcal{F} &= \frac{\tau}{i\mu} \{ \mathcal{F}, \mathcal{H} \} + i\sqrt{\tau} \sum_{jk} \left(\frac{\partial\mathcal{F}}{\partial\phi_j} G_{jk} \phi_k - \frac{\partial\mathcal{F}}{\partial\phi_k^*} G_{kj}^* \phi_j^* \right) \\ &\quad - \frac{\tau}{2} \sum_{jk} \left(\frac{\partial\mathcal{F}}{\partial\phi_j} K_{jk} \phi_k + \frac{\partial\mathcal{F}}{\partial\phi_k^*} K_{kj}^* \phi_j^* \right) \\ &\quad + \tau \sum_{jk\ell m} \frac{\partial^2\mathcal{F}}{\partial\phi_j \partial\phi_k^*} G_{j\ell} G_{km}^* \phi_\ell \phi_m^*. \end{aligned} \quad (35)$$

Taking the average of both sides of equation (35), the term proportional to $\sqrt{\tau}$ vanishes. After that, we divide what is left by τ to reach the result

$$\begin{aligned} \frac{d}{dt} \langle \mathcal{F} \rangle &= \frac{1}{i\mu} \langle \{ \mathcal{F}, \mathcal{H} \} \rangle - \sum_{jk\ell} \gamma_{\ell j, \ell k} \left(\langle \phi_k \frac{\partial\mathcal{F}}{\partial\phi_j} \rangle + \langle \phi_j^* \frac{\partial\mathcal{F}}{\partial\phi_k^*} \rangle \right) \\ &\quad + 2 \sum_{jk\ell m} \gamma_{km, j\ell} \langle \phi_\ell \phi_m^* \frac{\partial^2\mathcal{F}}{\partial\phi_j \partial\phi_k^*} \rangle. \end{aligned} \quad (36)$$

where here the average are taken over the probability density distribution \mathcal{P} , that is, the average $\langle \mathcal{F} \rangle$ of \mathcal{F} is

$$\langle \mathcal{F} \rangle = \int \mathcal{F} \mathcal{P} d\phi d\phi^*. \quad (37)$$

Taking into account that \mathcal{F} is an arbitrary function, we reach the equation for the time evolution of the probability distribution \mathcal{P} , which is

$$\begin{aligned} \frac{\partial \mathcal{P}}{\partial t} = & \frac{1}{i\mu} \{ \mathcal{H}, \mathcal{P} \} + \sum_{jkl} \gamma_{\ell j, \ell k} \left(\frac{\partial \phi_k \mathcal{P}}{\partial \phi_j} + \frac{\partial \phi_j^* \mathcal{P}}{\partial \phi_k^*} \right) \\ & + 2 \sum_{jklm} \gamma_{km, j\ell} \frac{\partial^2 \phi_\ell \phi_m^* \mathcal{P}}{\partial \phi_j \partial \phi_k^*}. \end{aligned} \quad (38)$$

To reach this equation we bear in mind that the averages in (36) are integrals in the complex vector space of the type (37). The expressions in (38) are found performing appropriate integrals by parts and considering that \mathcal{P} vanishes rapidly at the boundaries of integration. The equation (38) is recognized as a Fokker-Planck-Kramers equation [23–26], in several complex variables.

B. Master equation

The fundamental equation (38) was derived above considering a discrete time stochastic equation of motion and then taking the continuous time limit. Here we consider another derivation of the fundamental equation by considering a continuous time equation of motion but discretized variables ϕ and ϕ^* . To simplify the notation we write φ in the place of (ϕ, ϕ^*) and consider the following Kolmogorov equation, or master equation,

$$\frac{d}{dt} \mathcal{P}(\varphi) = \sum_{\varphi'} \{ W(\varphi, \varphi') \mathcal{P}(\varphi') - W(\varphi', \varphi) \mathcal{P}(\varphi) \}, \quad (39)$$

where $W(\varphi', \varphi)$ are the entries of a stochastic matrix W . A stochastic matrix holds two properties: 1) the off diagonal entries $W(\varphi', \varphi)$ are nonnegative and represent the probability rate of the transition $\varphi \rightarrow \varphi'$, and 2) it holds the property

$$\sum_{\varphi} W(\varphi, \varphi') = 0. \quad (40)$$

From these two properties, it follows from the Perron-Frobenius theorem that $\mathcal{P}(\varphi, t) \geq 0$ if at the initial time it holds this property, and it is normalized at all times,

$$\sum_{\varphi} \mathcal{P}(\varphi, t) = 1. \quad (41)$$

It is more convenient to construct the backward Kolmogorov equation, or adjoint master equation,

$$\frac{d}{dt} \mathcal{Q}(\varphi) = \sum_{\varphi'} W(\varphi, \varphi') \{ \mathcal{Q}(\varphi') - \mathcal{Q}(\varphi) \}. \quad (42)$$

We consider three types of transitions. The first is defined by

$$\phi_j \rightarrow \phi'_j = \phi_j + \frac{\varepsilon}{i\mu} H_{j\ell} \phi_\ell, \quad (43)$$

$$\phi_k^* \rightarrow \phi_k'^* = \phi_k^* - \frac{\varepsilon}{i\mu} H_{mk} \phi_m^*, \quad (44)$$

and occurs with rate one. The contribution of this transition to the right-hand side of equation (42) is given by the expression

$$\frac{1}{i\mu} \sum_{j\ell} \{ H_{j\ell} \phi_\ell \frac{\partial \mathcal{P}}{\partial \phi_j} - H_{\ell j} \phi_\ell^* \frac{\partial \mathcal{P}}{\partial \phi_j^*} \}. \quad (45)$$

The second type is defined by

$$\phi_j \rightarrow \phi'_j = \phi_j \pm i\sqrt{\varepsilon} g_{j\ell} \phi_\ell, \quad (46)$$

$$\phi_k^* \rightarrow \phi_k'^* = \phi_k^* \mp i\sqrt{\varepsilon} g_{km}^* \phi_m^*, \quad (47)$$

and occurs with transition rate $\alpha_{\ell m, jk} \geq 0$, which holds the property

$$\alpha_{\ell m, jk} = \alpha_{m\ell, kj}. \quad (48)$$

The contribution of this transition to the right-hand side of equation (42) is given by the expression

$$2 \sum_{jklm} \alpha_{\ell m, jk} \frac{\partial^2 \mathcal{Q}}{\partial \phi_j \partial \phi_k^*} g_{j\ell} \phi_\ell g_{km}^* \phi_m^*, \quad (49)$$

which is real due to the property (48).

The third type is defined by

$$\phi_j \rightarrow \phi'_j = \phi_j - \frac{1}{2} \varepsilon g_{\ell j}^* g_{\ell k} \phi_k, \quad (50)$$

$$\phi_k^* \rightarrow \phi_k'^* = \phi_k^* - \frac{1}{2} \varepsilon g_{\ell j} g_{\ell k}^* \phi_j^*, \quad (51)$$

occurring with rate $\alpha_{kj, \ell\ell} \geq 0$. The contribution of this transition to the right-hand side of equation (42) is given by the expression

$$- \sum_{\ell} \alpha_{kj, \ell\ell} g_{\ell j}^* g_{\ell k} \left\{ \frac{\partial \mathcal{Q}}{\partial \phi_j} \phi_k + \frac{\partial \mathcal{Q}}{\partial \phi_k^*} \phi_j^* \right\},$$

which is real due to the property (48).

Replacing the expressions obtained above in the right-hand side of equation (42), it becomes identical to the adjoint equation (36), if we set

$$\gamma_{km, j\ell} = \alpha_{\ell m, jk} g_{j\ell} g_{km}^*. \quad (52)$$

Taking into account that $\gamma_{km, j\ell}$ is the covariance $\langle G_{km}^* G_{j\ell} \rangle$, then the random variables G_{jk} must obey the relation

$$\langle G_{km}^* G_{j\ell} \rangle = \alpha_{\ell m, jk} g_{j\ell} g_{km}^*. \quad (53)$$

This is accomplished if the absolute value of G_{jk} is a random variable but not its phase. Indeed, if we write $G_{jk} = R_{jk} e^{ia_{jk}}$ then

$$\langle G_{km}^* G_{j\ell} \rangle = \langle R_{km} R_{j\ell} \rangle e^{-ia_{km}} e^{ia_{j\ell}}, \quad (54)$$

which is of the form (53).

C. Central equation

Equation (38) that governs the time evolution of the probability density distribution $\mathcal{P}(\phi, \phi^*)$ is the fundamental equation of the present stochastic approach. From this equation we derive the equation for the time evolution of any bilinear state function such as the covariances $\rho_{jk} = \langle \phi_j \phi_k^* \rangle$ of the stochastic variables ϕ_j . The equation that give the time evolution of ρ_{jk} is obtained from (38) but we may as well use the equation (36) by replacing \mathcal{F} by $\phi_j \phi_k^*$. The result is

$$\begin{aligned} \frac{d}{dt} \rho_{jk} &= \frac{1}{i\mu} \sum_{\ell} (H_{j\ell} \rho_{\ell k} - \rho_{j\ell} H_{\ell k}) \\ &- \sum_{\ell m} (\gamma_{mj, m\ell} \rho_{\ell k} + \rho_{j\ell} \gamma_{m\ell, mk}) + 2 \sum_{\ell m} \gamma_{km, j\ell} \rho_{\ell m}. \end{aligned} \quad (55)$$

Once this equation is solved, the average $\langle \mathcal{F} \rangle$ of a bilinear function \mathcal{F} is obtained by

$$\langle \mathcal{F} \rangle = \sum_{jk} F_{jk} \rho_{kj}. \quad (56)$$

Equation (55) is the central equation of the present approach and is the most general form of an equation for the covariance ρ_{jk} that can be derived from a noise that is linear in ϕ_j and which conserves in the average the norm of ϕ_j . The coefficients $\gamma_{\ell j, km}$ are not arbitrary. As mentioned above, $\gamma_{\ell j, km}^* = \gamma_{km, \ell j}$ and the eigenvalues of the $n^2 \times n^2$ matrix with elements $\gamma_{\ell j, km}$ are nonnegative.

The central equation (55) can be written in matrix form as follows. We first define the covariance matrix ρ as the $n \times n$ matrix with elements ρ_{jk} . Then we introduce $n \times n$ matrices A^{jk} whose entries are all zero except the entry at row j and column k which equals 1. Notice that A^{jk} is not an entry of a matrix but denotes one of a collection of n^2 matrices. Their entries are denoted by $A_{\ell m}^{jk}$ and are given by

$$A_{\ell m}^{jk} = \delta_{j\ell} \delta_{km}. \quad (57)$$

The matrices A^{jk} form a complete basis for the expansion of any $n \times n$ matrix. For instance, in terms of this set the matrix ρ has the expansion

$$\rho = \sum_{jk} \rho_{jk} A^{jk}. \quad (58)$$

In terms of the basis matrices, the central equation (55) becomes

$$\begin{aligned} \frac{d\rho}{dt} &= \frac{1}{i\mu} [H, \rho] \\ &+ \sum_{jk\ell m} \gamma_{jk, \ell m} (2A^{\ell m} \rho A^{jk\dagger} - A^{jk\dagger} A^{\ell m} \rho - \rho A^{jk\dagger} A^{\ell m}), \end{aligned} \quad (59)$$

where $[H, \rho] = H\rho - \rho H$ stands for the commutation between the matrices H and ρ .

Using (56), the average of $\langle \mathcal{F} \rangle$ of a bilinear state function \mathcal{F} is determined from ρ by

$$\langle \mathcal{F} \rangle = \text{Tr} F \rho. \quad (60)$$

The matrix ρ holds the following properties. It is a Hermitian matrix with unit trace,

$$\text{Tr} \rho = 1, \quad (61)$$

and is a semi-positive definite matrix, which means that its eigenvalues are non-negative. These properties, which allow us to call ρ a density matrix, follow from the definition of ρ as a covariance matrix, that is,

$$\rho_{jk} = \int \phi_j \phi_k^* \mathcal{P} d\phi d\phi^*, \quad (62)$$

and from the properties of the distribution density which are $\mathcal{P} \geq 0$ and normalization,

$$\int \mathcal{P} d\phi d\phi^* = 1. \quad (63)$$

The Hermitian property $\rho_{jk}^* = \rho_{kj}$ follows from (62). As ρ is Hermitian its eigenvalues are real. To show that the eigenvalues are nonnegative it suffices to consider a transformation that diagonalizes ρ and use this transformation to change the variables ϕ_j to new variables ϕ'_j . Taking into account that $\rho_{jk} = \langle \phi_j \phi_k^* \rangle$ then $\langle \phi'_j \phi'^*_k \rangle$ will be diagonal and coincides with the eigenvalues p_j of ρ . Therefore, $p_j = \langle \phi'_j \phi'^*_j \rangle \geq 0$.

The fundamental equation was construct in such a way that the norm was conserved in the average, which means that

$$\langle \mathcal{N} \rangle = \sum_j \rho_{jj} \quad (64)$$

is constant. Choosing this constant to be equal to unity, then $\text{Tr} \rho = 1$. Alternatively, it follows from equation (59) that $d\text{Tr} \rho / dt = 0$. The semi-definite property of ρ is also preserved at all times because at any time ρ_{jk} keeps being a covariance.

The above properties are valid as long as \mathcal{P} conserves the properties of a probability density distribution stated above. But this is indeed the case as we have demonstrated above.

The equation (59) is formally identical to the quantum master equation [27, 28] introduced by Lindblad [29] and by Gorini, Kossakowski, and Sudarshan [30], describing the time evolution of a density matrix of a quantum open system. The distinguish feature between them is that equation (59) was obtained by considering that ρ is a covariance matrix. Of course, as we have shown above, it turned out to be a density matrix.

It is worth considering the time evolution of the average $\chi_j = \langle \phi_j \rangle$. From (36) we find

$$\frac{d\chi_j}{dt} = \frac{1}{i\mu} \sum_k H_{jk} \chi_k - \frac{1}{2} \sum_k \gamma_{jk} \chi_k, \quad (65)$$

where $\gamma_{jk} = \langle K_{jk} \rangle$.

IV. QUANTUM MECHANICS

The noise defined by the last two terms of (24) changes the variable ϕ_j by changing both the phase θ_j and the absolute value r_j of $\phi_j = r_j e^{i\theta_j}$. However, if the noise is of the type given by the equation

$$\Delta\phi_j = (i\sqrt{\tau}\xi - \frac{\tau}{2}\gamma)\phi_j, \quad (66)$$

where ξ is a random variable with zero mean and variance γ , then the noise still changes the phase θ_j but not the absolute value of ϕ_j . To show this result it suffices to write this equation in the equivalent form

$$\phi'_j = e^{i\sqrt{\tau}\gamma\xi}\phi_j, \quad (67)$$

where $\phi'_j = \phi_j + \Delta\phi_j$. This result shows that $\phi_j^* \phi_j = r_j^2$ is invariant and the norm \mathcal{N} is conserved in the strict sense.

The noise defined by the expression (66) corresponds to set $2\gamma_{j\ell, km} = \gamma\delta_{j\ell}\delta_{km}$. The equation (36) reduces to

$$\begin{aligned} \frac{d}{dt}\langle\mathcal{F}\rangle &= \frac{1}{i\mu}\langle\{\mathcal{F}, \mathcal{H}\}\rangle \\ &- \frac{1}{2}\gamma\sum_j\langle\phi_j\frac{\partial\mathcal{F}}{\partial\phi_j} + \phi_j^*\frac{\partial\mathcal{F}}{\partial\phi_j^*}\rangle + \gamma\sum_{jk}\langle\phi_j\phi_k^*\frac{\partial^2\mathcal{F}}{\partial\phi_j\partial\phi_k^*}\rangle, \end{aligned} \quad (68)$$

and the fundamental equation (38) becomes

$$\begin{aligned} \frac{d\mathcal{P}}{dt} &= \frac{1}{i\mu}\{\mathcal{H}, \mathcal{P}\} \\ &+ \frac{\gamma}{2}\sum_j\left(\frac{\partial\phi_j}{\partial\phi_j}\mathcal{P} + \frac{\partial\phi_j^*}{\partial\phi_j^*}\mathcal{P}\right) + \gamma\sum_{jk}\frac{\partial^2\phi_j\phi_k^*\mathcal{P}}{\partial\phi_j\partial\phi_k^*}, \end{aligned} \quad (69)$$

which reduces to the simpler form

$$\frac{\partial\mathcal{P}}{\partial t} = \frac{1}{i\mu}\{\mathcal{P}, \mathcal{H}\} + \gamma^2\sum_{jk}\frac{\partial^2\mathcal{P}}{\partial\theta_j\partial\theta_k}. \quad (70)$$

In this case the equation (55) becomes

$$\frac{d}{dt}\rho_{jk} = \frac{1}{i\mu}\sum_{\ell}(H_{j\ell}\rho_{\ell k} - \rho_{j\ell}H_{\ell k}), \quad (71)$$

which can be written in the matrix form as

$$\frac{d\rho}{dt} = \frac{1}{i\mu}[H, \rho], \quad (72)$$

which is the quantum Liouville equation, if we set $\mu = \hbar$. The equation (65) for χ_j becomes

$$\frac{d\chi_j}{dt} = \frac{1}{i\mu}\sum_k H_{jk}\chi_k - \frac{1}{2}\gamma\chi_j. \quad (73)$$

We remark that the equation (71) does not have the terms corresponding to the noise. However, this does not mean that the effect of the noise is not present. The variable ϕ_j is still a stochastic variable which is reflected in the last term of equation (73).

The equation (71) has a special type of solution which is $\rho_{jk} = \psi_j\psi_k^*$. Replacing this form of ρ in the equation (71), we see that it is indeed a solution as long as ψ_j fulfills the equation

$$\frac{d\psi_j}{dt} = \frac{1}{i\mu}\sum_k H_{jk}\psi_k, \quad (74)$$

or in matrix form

$$\frac{d\psi}{dt} = \frac{1}{i\mu}H\psi, \quad (75)$$

where ψ is a column matrix with elements ψ_j , and

$$\rho = \psi\psi^\dagger, \quad (76)$$

where ψ^\dagger is a row matrix with elements ψ_j^* . A solution of this type is called pure state and equation (75) is identified as the Schrödinger equation, if we set $\mu = \hbar$. We remark that ψ_j should not be confused with ϕ_j nor with $\chi_j = \langle\phi_j\rangle$. This last quantity obeys the equation (73) which differs from (74) by the presence of the term $-\gamma\chi_j/2$ which makes χ_j to vanish in the long term.

The relation between ϕ_j and ψ_j is

$$\psi_j\psi_k^* = \langle\phi_j\phi_k^*\rangle = \rho_{jk}, \quad (77)$$

and in particular

$$|\psi_j|^2 = \langle|\phi_j|^2\rangle = \rho_{jj}. \quad (78)$$

Due to the invariance of the norm given by (64) it follows the usual normalization of ψ_j ,

$$\sum_j |\psi_j|^2 = 1. \quad (79)$$

The average $\langle\mathcal{F}\rangle$ given by equation (56) now reads

$$\langle\mathcal{F}\rangle = \sum_{jk}\psi_k^* F_{jk}\psi_j, \quad (80)$$

which is the usual expression for the quantum average.

V. QUANTUM THERMODYNAMICS

A. First law of thermodynamics

We start by writing the central equation (59) in a more convenient form as follows

$$\frac{d\rho}{dt} = \frac{1}{i\mu}[H, \rho] + L, \quad L = \sum_r L^r \quad (81)$$

where

$$L^r = \frac{1}{2} \sum_s \{ \gamma_{r,s} [A^s \rho, A^{r\dagger}] + \gamma'_{r,s} [A^s \rho, A^r] + \gamma_{r,s}^* [A^r, \rho A^{s\dagger}] + \gamma'^*_{r,s} [A^{r\dagger}, \rho A^{s\dagger}] \}, \quad (82)$$

and we are using a convention concerning the index notation defined by the replacements $jk \rightarrow r$ and $\ell m \rightarrow s$, and $\gamma'_{jk,\ell m} = \gamma_{kj,\ell m}$, and we remark that $L^{r\dagger} = L^r$. Defining the auxiliary matrices

$$B^r = \sum_s \gamma_{rs} A^s, \quad C^r = \sum_s \gamma'_{r,s} A^s, \quad (83)$$

then L^r acquires the simpler form

$$L^r = \frac{1}{2} \{ [A^r, \rho B^{r\dagger} - C^r \rho] - [A^{r\dagger}, B^r \rho - \rho C^{r\dagger}] \}. \quad (84)$$

Notice that $B_{\ell m}^{jk} = \gamma_{jk,\ell m}$ and $C_{\ell m}^{jk} = \gamma_{kj,\ell m}$.

From the central equation (81) we determine the equation that gives the time evolution of the average $\langle \mathcal{F} \rangle = \text{Tr}(F\rho)$ of a bilinear state function. It is given by

$$\frac{d\langle \mathcal{F} \rangle}{dt} = \frac{1}{i\mu} \text{Tr} F[H, \rho] + \sum_r \text{Tr} F L^r. \quad (85)$$

In accordance with thermodynamics the change in the energy \mathcal{E} of an open system equals the heat introduced into the system minus the work done by the system on the environment, which is the law of conservation of energy, or the first law of thermodynamics. The work is assumed to be the increment in a potential \mathcal{V} due to the external forces. The conservation of energy is then written as

$$\frac{d\langle \mathcal{E} \rangle}{dt} = \Phi - \frac{d\langle \mathcal{V} \rangle}{dt}, \quad (86)$$

where Φ is the flux of heat into the system. We assume that the Hamiltonian function \mathcal{H} is the sum of the energy function \mathcal{E} and the potential \mathcal{V} of the external forces, $\mathcal{H} = \mathcal{E} + \mathcal{V}$. Bearing this in mind, we write

$$\frac{dU}{dt} = \Phi, \quad (87)$$

where $U = \langle \mathcal{H} \rangle$.

To determine the expression of Φ , we calculate the left-hand side of equation (87) using equation (85). The result for the flux is

$$\Phi = \sum_r \Phi_r, \quad (88)$$

where

$$\Phi_r = \text{Tr} H L^r. \quad (89)$$

Equation (87), with Φ representing the total flux of heat into the system, expresses the conservation of energy, or the first law of thermodynamics.

B. Second law of thermodynamics

If we wish to describe an open system regarded as a thermodynamic system in the sense that it obeys the laws of thermodynamics we need to introduce two quantities which are the entropy S of the system and the flux of entropy Ψ .

Let $f(x) \leq 0$ be a decreasing and convex function of x defined on the interval $0 \leq x \leq 1$, and such that $f(1) = 0$. We also require that $xf(x) \rightarrow 0$ when $x \rightarrow 0$. An example of $f(x)$ holding these properties is the function $-\ln x$. The entropy S of the system is then defined by

$$S = \kappa \sum_j p_j f(p_j), \quad (90)$$

where κ is some positive constant and $p_j \geq 0$ are the eigenvalues of the matrix ρ , which are subject to the condition

$$\sum_j p_j = 1, \quad (91)$$

following from $\text{Tr} \rho = 1$.

Considering that $0 \leq p_j \leq 1$ it follows that $S \geq 0$. The minimum value of the entropy is $S = 0$ which occurs when one of the quantities p_j equals one, which is the case of pure states. In terms of the matrix ρ , the entropy can be written as

$$S = \kappa \text{Tr} \rho f(\rho). \quad (92)$$

Deriving S with respect to time and using the central equation (81), we find

$$\frac{dS}{dt} = \kappa \sum_r \text{Tr} L^r f(\rho). \quad (93)$$

By calling S the entropy we wish that it describes the thermodynamic entropy. A distinguishing property of thermodynamic entropy is that it is not a conserved quantity. For instance, a system that has its energy increased only because of heat flow must have its entropy increased. Therefore, the right-hand side of (93) is not in general the entropy flux.

Concerning the entropy flux, we assume with Clausius that the entropy flux is the ratio between the heat flux and the temperature of the environment. More precisely, we assume that the total entropy flux is a sum of entropy fluxes coming from distinct parts of the environment which are at distinct temperatures. The entropy flux Ψ_r coming from the r -th part of the environment at temperature T_r is

$$\Psi_r = \frac{\Phi_r}{T_r}, \quad (94)$$

where Φ_r is the heat flux coming from the r -th part which we assume to be given by the expression (89). However, we cannot adopt the Clausius relation in the strict sense

because no temperature has yet been defined. But we can still assume the Clausius relation, with the understanding that $T_r > 0$ are parameters of the present approach.

Replacing the expression for the heat flux given by (89) in (94), we find the desired expression for the flux of entropy coming from the r -th part of the environment,

$$\Psi_r = \frac{1}{T_r} \text{Tr} H L^r. \quad (95)$$

The total flux of entropy is

$$\Psi = \sum_r \Psi_r. \quad (96)$$

The right-hand side of (93) must be the sum of the entropy flux Ψ from the environment and another term corresponding to the creation of entropy which is the rate of entropy production Π within the system, defined by

$$\frac{dS}{dt} = \Pi + \Psi, \quad (97)$$

From this relation we determine Π using the expressions of the flux of entropy Ψ and dS/dt . Before that, we define ρ^r through the relation

$$\beta_r H = f(\rho^r) + c_r, \quad (98)$$

where c_r is such that $\text{Tr} \rho_r = 1$, and $\beta_r = 1/\kappa T_r$. From this relation and equation (95) we may write Ψ_r as

$$\Psi_r = \kappa \text{Tr} L^r f(\rho^r), \quad (99)$$

where the constant C_r has disappeared because $\text{Tr} L^r = 0$. Subtracting (99) from (93), we find

$$\Pi = \kappa \sum_r \text{Tr} L^r \{f(\rho) - f(\rho^r)\}. \quad (100)$$

According to Clausius the increase in the entropy S of a system is larger than or equal to the entropy flux Ψ into the system,

$$\frac{dS}{dt} \geq \Psi, \quad (101)$$

which constitutes the second law of thermodynamics. Taking into account the equality (97), the Clausius expression (101) of the second law can be written in the equivalent form

$$\Pi \geq 0. \quad (102)$$

In the following, we will demonstrate this inequality proving thus the Clausius expression for the second law of thermodynamics.

C. Positivity of the entropy production

To show that $\Pi \geq 0$, we demonstrate that each term of the summation in (100) is nonnegative, that is, we demonstrate that $\Pi_r \geq 0$,

$$\Pi_r = \kappa \text{Tr} L^r(\rho) \{f(\rho) - f(\rho^r)\}, \quad (103)$$

and L^r is given by (84).

Our procedure is to show (a) that Π_r is a convex function of the eigenvalues p_ℓ of ρ , and (b) that Π_r is bounded from below at $\rho = \rho^r$, in which case $\Pi_r = 0$. If the first proposition is demonstrated, then the second proposition can be met if $\rho = \rho^r$ is a double zero of Π_r which amounts to say that L^r vanishes when $\rho = \rho^r$. This condition leads consistently to the vanishing of Ψ_r as well. The vanishing of L^r is fulfilled by demanding that

$$B^r \rho^r = \rho^r C^{r\dagger}, \quad (104)$$

which we assume from now on. As B^r and C^r are defined in terms of $\gamma_{r,s}$ and ρ^r depends on T_r , this condition establishes a relation between the correlations $\gamma_{r,s}$ and the parameter T_r .

To show that Π_r is convex it suffices to show that

$$R_r = \text{Tr} L^r(\rho) f(\rho) \quad (105)$$

is convex because $L^r(\rho)$ is linear in ρ . We provide the demonstration of convexity of R_r for the case in which $L(\rho)$ has a diagonal form, which is equivalent to express $L^r(\rho)$ as

$$L^r = \frac{\lambda_r}{2} \{[A^r, [\rho, A^{r\dagger}]] + [A^{r\dagger}, [\rho, A^r]]\}, \quad (106)$$

in which case

$$R_r = \lambda_r \Re \text{Tr} \{[f, A^{r\dagger} \rho] A^r + [f, A^r \rho] A^{r\dagger}\}. \quad (107)$$

Next, we consider the following term of R_r ,

$$\text{Tr} [f, A \rho] A^\dagger, \quad (108)$$

where for simplicity we have dropped the index of A^r , and we observe that it is the limit when $\varepsilon \rightarrow 0$ of the expression

$$\frac{1}{\varepsilon} \text{Tr} \{e^{\varepsilon f} A \rho e^{-\varepsilon f} A^\dagger - A \rho A^\dagger\}. \quad (109)$$

The expression (108) is convex if the first term of (109) is convex as the second term is linear in ρ . To see that this is the case it suffices to write it in the following symmetric form

$$\text{Tr} \{(e^{\varepsilon f/2} A \rho^{1/2} e^{-\varepsilon f/2}) (e^{-\varepsilon f/2} \rho^{1/2} A^\dagger e^{\varepsilon f/2})\}. \quad (110)$$

In the general case, instead of terms of the type (108), we face terms of the type

$$\text{Tr} [f, A^r \rho] B^{r\dagger}, \quad (111)$$

which is equal to

$$\sum_s \gamma_{rs}^* \text{Tr}[f, A^r \rho] A^{s\dagger}. \quad (112)$$

We then expand A^r in another basis set A'^s in such a way that the expression (112) becomes diagonal in A'^s , that is,

$$\sum_s \lambda_s \text{Tr}[f, A'^s \rho] A'^{s\dagger}. \quad (113)$$

Now each of the terms of the summation is similar to (108) and we may apply the same reasoning above to show that it is convex. This concludes the demonstration that $\Pi_r \geq 0$ and $\Pi \geq 0$.

VI. FOKKER-PLANCK-KRAMERS STRUCTURE

A. Fluctuation and dissipation

The classical Fokker-Planck-Kramers (FPK) equation describes a massive particle under the action of a conservative force plus, a dissipative force, and a fluctuating force [23, 26]. These forces give rise to three terms in the equation which are the Hamiltonian part, the dissipative part, and the fluctuation part. In the following we show that the central equation has a similar structure and can thus be understood as the quantum version of the FPK equation.

From the expressions (81) and (84), the central equation can be written in the form

$$i\mu \frac{d\rho}{dt} = [H, \rho] - \sum_r [A^r, J^{r\dagger}], \quad (114)$$

where J^r is the current, given by

$$J^r = i\mu(B^r \rho - \rho C^{r\dagger}). \quad (115)$$

Defining $D^r = B^{r\dagger} - C^r$, the current becomes

$$J^r = i\mu(D^{r\dagger} \rho - [\rho, C^{r\dagger}]). \quad (116)$$

Replacing it in (114), the central equation, it acquires the form

$$i\mu \frac{d\rho}{dt} = [H, \rho] + i\mu \sum_r [A^r, \rho D^{r\dagger}] - i\mu \sum_r [A^r, [C^r, \rho]], \quad (117)$$

which has the form of the FPK equation. The three terms on the right-hand side are respectively, the Hamiltonian part, the dissipative part, and the fluctuation part.

Using the relation (104), we find the following form for the term related to the dissipation,

$$D^r = (\rho^r)^{-1} C^r \rho^r - C^r. \quad (118)$$

Therefore, the equation (114) can be set up if we are given C^r and ρ^r .

B. Detailed balance

The stationary solution ρ^{st} of the central equation (114) is determined by

$$[H, \rho^{\text{st}}] - \sum_r [A^r, J^{r\dagger}(\rho^{\text{st}})] = 0. \quad (119)$$

Depending on the covariances of the independent random variables, that is, on B^r and C^r , the stationary solution may in addition obey a detailed balance condition. Denoting in this case the stationary solution by ρ^e , the detailed balance condition is equivalent to say that each term of (119) vanishes, that is, $[H, \rho^e] = 0$ and $J^{r\dagger}(\rho^e) = 0$, or

$$B^r \rho^e = \rho^e C^{r\dagger}. \quad (120)$$

for all r , which is the expression of the detailed balance condition. This solution is understood as describing the thermodynamic equilibrium, understood as the state devoid of currents.

We remark that the detailed balance condition (120) should not be confused with the relation (104) between B^r and $C^{r\dagger}$. If we use relation (104), the detailed balance condition is just $\rho^e = \rho^r$, for all r . Bearing in mind that the expression of ρ^r for distinct r has the same form given by equation (98), differing only on the parameter T_r , we see that the detailed balance condition occurs if all the parameters $T_r = T$ are equal. In this case we may identify the common value T as the temperature of the system and the ρ^e is given by $\beta H = f(\rho^e) + c$, or

$$\rho^e = f^{-1}(\beta H - c), \quad (121)$$

where f^{-1} is the function inverse of f . We recall that the function f is related to the entropy by $S = \kappa \text{Tr} f(\rho)$.

If $f = -\ln x$, in which case the entropy is given by $S = -\kappa \text{Tr} \rho \ln \rho$, then $f^{-1} = e^{-x}$ and

$$\rho^e = \frac{1}{Z} e^{-\beta H}, \quad (122)$$

where $\beta = 1/\kappa T$, which is the Gibbs equilibrium state for a system at a temperature T .

C. Non-equilibrium stationary states

Writing L^r in terms of the current J^r , the expression for the heat flux Φ_r , the entropy flux $\Psi_r = \Phi_r/T_r$, and the rate of entropy Π_r are given by

$$\Phi_r = \frac{1}{i\mu} \text{Tr} J^{r\dagger} [A^r, H], \quad (123)$$

$$\Psi_r = \frac{\kappa}{i\mu} \text{Tr} J^{r\dagger} [A^r, f(\rho^r)], \quad (124)$$

$$\Pi_r = \frac{\kappa}{i\mu} \text{Tr} J^{r\dagger} [A^r, f(\rho) - f(\rho^r)]. \quad (125)$$

The total heat flux, the total entropy flux and the total entropy rate are

$$\Phi = \sum_r \Phi_r, \quad (126)$$

$$\Psi = \sum_r \Psi_r = \sum_r \frac{1}{T_r} \Phi_r, \quad (127)$$

$$\Pi = \sum_r \Pi_r. \quad (128)$$

In the stationary state Φ and $\Pi + \Psi$ vanish. If in addition the thermodynamic equilibrium is established, which occurs if all T_r are equal, then all currents J^r vanish. In this case Φ_r , Ψ_r , and Π_r as well as Π and Ψ also vanish. If the stationary state is not an equilibrium state, which occurs if at least of T_r is distinct from the others, then at least one of the currents J^r are nonzero. In this case, Π and Ψ are nonzero, although their sum vanishes. As $\Pi \geq 0$, then in the nonequilibrium stationary state

$$\Pi = -\Psi > 0. \quad (129)$$

D. Examples

We have proposed a quantum FPK equations which was obtained through the canonical quantization [34]. For a system of quantum particles of mass m the quantum FPK equation reads [34]

$$\begin{aligned} i\hbar \frac{\partial \rho}{\partial t} = & [H, \rho] + \frac{1}{2} \sum_j \gamma_j [x_j, \rho g_j + g_j^\dagger \rho] \\ & + \frac{\gamma_j m}{i\hbar \beta_j} \sum_j [x_j, [x_j, \rho]], \end{aligned} \quad (130)$$

where x_j represents the position of particle j , and

$$g_j = -\frac{m}{i\hbar \beta_j} (e^{\beta_j H} x_j e^{-\beta_j H} - x_j).$$

We see that this equation has the form of equation (104) if we set $\mu = \hbar$, $A_j = x_j$,

$$C_j = \frac{\gamma_j m}{\hbar^2 \beta_j} x_j, \quad \text{and} \quad D_j = \frac{\gamma_j g_j}{2i\hbar}. \quad (131)$$

The expansion of g_j gives

$$g_j = p_j + \frac{\beta_j}{2!} [H, p_j] + \frac{\beta_j^2}{3!} [H, [H, p_j]] + \dots \quad (132)$$

where p_j is the momentum of particle j . As g_j is related to dissipation we see that the quantum friction is not generally proportional to the momentum as is the case of the classical case, as is manifest in the classical FPK equation.

For bosons the canonical quantization leads to the following equation [35, 36]

$$\begin{aligned} i\hbar \frac{\partial \rho}{\partial t} = & [H, \rho] + i\gamma_j \sum_j \{[a_j, \rho g_j^\dagger] - [a_j^\dagger, g_j \rho]\} \\ & - \frac{i\gamma_j}{\beta_j} \sum_j \{[a_j, [a_j^\dagger, \rho]] + [a_j^\dagger, [a_j, \rho]]\}, \end{aligned} \quad (133)$$

where a_j and a_j^\dagger represent, respectively, the annihilation and creation of a boson in a one-particle state labeled by the index j , and

$$g_j = \frac{1}{\beta_j} (e^{-\beta_j H_j} a_j e^{\beta_j H_j} - a_j). \quad (134)$$

Again we see that this equation has the form of equation (104), if we set $\mu = \hbar$, $A_j = a_j$,

$$C_j = \frac{\gamma_j}{\hbar \beta_j} a_j, \quad \text{and} \quad D_j = \frac{\gamma_j}{\hbar} g_j.$$

VII. CONCLUSION

We have derived the equations of quantum mechanics and quantum thermodynamics from the assumption that a quantum system can be described by an underlying classical system of particles. Each component ϕ_j of the wave vector ϕ is understood as a complex variable whose real and imaginary parts are proportional to the coordinate and momentum associated to a degree of freedom of the underlying classical system. The equation of motion is considered to be a stochastic equation so that ϕ_j is a stochastic variable. This result leads us to conclude that the density matrix ρ obeying either the quantum Liouville or the Lindblad equation is the covariance matrix associated to the random wave vector ϕ . In this sense the present approach gives a meaning to the off-diagonal terms of ρ .

The understanding of the wave vector ϕ as a stochastic variable and ρ as its covariance matrix allows an interpretation of quantum mechanics other than the standard interpretation [20–22]. As the trajectory in the Hilbert space are stochastic the present approach may fit the consistent history interpretation of quantum mechanics [8] since the several trajectories are possible, each one occurring with a certain probability. The present approach is also in accordance with the standard interpretation if we bear in mind that $\text{Tr} \rho = 1$, which means that ρ_{ii} can be interpreted as a probability.

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