STATISTICAL

Quantum Fokker-Planck Structure of the Lindblad Equation

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Abstract

We show that the quantum Fokker-Planck equation, obtained by a canonical quantization of its classical version, can be transformed into an equation of the Lindblad form. This result allows us to conclude that the quantum Fokker-Planck equation preserves the trace and positivity of the density operator. The Fokker-Planck structure gives explicit expression for the quantum equivalence of probability current as well as the quantum equivalence of detailed balance. We also propose expression for the rate of entropy production and show that it does not vanish for a closed system except in equilibrium.

Keywords Quantum Fokker-Planck equation · Lindblad equation · Stochastic thermodynamics

1 Introduction

The dynamics of quantum open systems [1–16] is usually formulated considering a system and its environment. The equation of motion of the system is then derived by summing out the degrees of freedom of the environment. The derivation is not accomplished without assuming an approximation concerning the interactions of the system with its environment. Usually, the environment is considered a thermal system which means to say that the interaction with the system is regarded as being of stochastic nature.

Starting from the quantum Liouville equation for the total system, which is the system proper and its environment, the resulting evolution equation is a quantum Liouville equation supplemented by a dissipation term D [14–16],

$$\frac{d\rho}{dt} = \frac{1}{i\hbar}[H, \rho] + D,$$ (1)

where H is the Hamiltonian of the system.

Taking into account that the variables of the environment act as stochastic variables, the reduced Eq. (1) describes a quantum Markov process which means that the dynamics is described by a quantum dynamic semi-group. The most general form of the generator D that has the property of

semi-group and that preserves the trace and positivity of the density operator is of the Lindblad form [14–16],

$$D = \sum_{jk} a_{jk}(2A_j\rho A_k^\dagger - A_k^\dagger A_j\rho - \rho A_k^\dagger A_j),$$ (2)

where a_{jk} are the entries of a Hermitian and positive matrix. The Eq. (1) with D in the form (2) is called the Lindblad equation.

An alternative approach to reach an equation for quantum open system is to consider the classical Fokker-Planck-Kramers equation [17–20], which is known to describe open classical systems, and carry out its canonical quantization. This approach has been indeed carried out by the present author [21, 22]. The resulting quantum Fokker-Planck (FP) equation was then applied to a system of two harmonic oscillators in contact with heat reservoirs at distinct temperatures from which the quantum thermal conductance was determined [21]. It was also used to calculate the thermal conductance of a two-level atom coupled to quantum oscillators [23], and to study the heat transport along a chain of coupled quantum oscillators [24] and of a bosonic system [25].

The quantum Fokker-Planck (FP) equation resulting from the canonical quantization is given by [21]

$$i\hbar\frac{d\rho}{dt} = [H, \rho] - \frac{1}{2}\sum_j [x_j, J_j + J_j^\dagger],$$ (3)

where J_j is the quantum version of the probability current, given by

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$$J_j = -\gamma_j(\rho g_j + \frac{m}{i\hbar\beta_j}[x_j, \rho]), \tag{4}$$

and

$$g_j = -\frac{m}{i\hbar\beta_j}(e^{\beta_j H} x_j e^{-\beta_j H} - x_j). \tag{5}$$

As happens to its classical version, this equation describes the contact of a system of interacting particles of mass m with thermal reservoirs at temperatures inversely proportional to β_j, and γ_j measures the strength of the interaction with the reservoirs. The positions and momenta of the particles are denoted by x_j and p_j. The first and second terms of the current J_j correspond to the dissipation and fluctuation, respectively. We remark that g_j, which is related to dissipation, is not in general proportional to the momentum p_j as in the classical dissipation but becomes proportional to p_j in the classical limit.

Equations similar to (3) were considered by Dekker [5] and by Caldeira and Leggett [8, 15]. However, there is a difference in that the dissipation term of their equations is proportional to the momentum whereas in Eq. (3), the dissipation term is proportional to a general term g_j which depends on the Hamiltonian of the system as can be seen in Eq. (5). This form of g_j is crucial if we wish to describe the thermodynamic equilibrium, or in other words, if we wish that the system thermalizes in the long run.

The quantum FP Eq. (3) can be written in a more symmetric form in terms of annihilation and creation operator a_j and $a_j^\dagger$ in which case it reads

$$i\hbar\frac{d\rho}{dt} = [H, \rho] - \sum_j([a_j, J_j^\dagger] + [a_j^\dagger, J_j]), \tag{6}$$

where

$$J_j = i\gamma_j(g_j\rho + \frac{1}{\beta_j}[a_j, \rho]), \tag{7}$$

and

$$g_j = \frac{1}{\beta_j}(e^{-\beta H} a_j e^{\beta_j h} - a_j). \tag{8}$$

It is worth writing J_j in the form

$$J_j = \frac{i\gamma_j}{\beta_j}(e^{-\beta H} a_j e^{\beta_j h} \rho - \rho a_j). \tag{9}$$

The quantum FP equation in either forms (3) or (6) is understood as describing a quantum Markov process and in this sense it should be of the type given by Eqs. (1) and (2). The first term of the quantum FP equation which corresponds to a unitary transformation is indeed the same. As to the second non-unitary term, it is not of the Lindblad type

given by (2). The main purpose of the present paper is to show that the second term of the quantum FP equation can be transformed into the Lindblad form, showing thus that the quantum FP equation preserves the trace and positivity of the density operator ρ.

2 Quantum FP Structure

We consider a Hilbert vector space and choose a basis consisting of the eigenvectors of some Hermitian operator L. The eigenvectors associated to the eigenvalue λ_i of L are denoted by ϕ_i, that is, $L\phi_i = \lambda_i\phi_i$. Taking into account that L is Hermitian its left eigenvectors are the adjoint vector $\phi_i^\dagger$. The operators acting on the vectors of the Hilbert space such as L itself can also be understood as belonging to another vector space, the Liouville space, whose complete basis consists of the operators $A_{ij} = \phi_j\phi_i^\dagger$.

The general expression of a non-unitary generator D which preserve the trace of ρ and its complete positivity for any initial condition is of the Lindblad form [14],

$$D = \sum_{ij,k\ell} a_{ij,k\ell}(2A_{ij}\rho A_{k\ell}^\dagger - A_{k\ell}^\dagger A_{ij}\rho - \rho A_{k\ell}^\dagger A_{ij}), \tag{10}$$

where $a_{ij,k\ell}$ are the entries of a Hermitian and positive matrix. Our point of depart is the following expression of the Lindblad type

$$\begin{aligned}
D = &\sum_{ij,k\ell} b_{ij,k\ell}(2A_{ij}\rho A_{k\ell}^\dagger - A_{k\ell}^\dagger A_{ij}\rho - \rho A_{k\ell}^\dagger A_{ij}) \\
&+ \sum_{ij,k\ell} c_{ij,k\ell}(2A_{ij}^\dagger\rho A_{k\ell} - A_{k\ell}A_{ij}^\dagger\rho - \rho A_{k\ell}A_{ij}^\dagger),
\end{aligned} \tag{11}$$

where $b_{ij,k\ell}$ and $c_{ij,k\ell}$ are the entries of Hermitian and positive matrices, and are nonzero only when $i \leq j$ and $k \leq \ell$.

Defining the operators B_{ij} by

$$\alpha_{ij}B_{ij} = \sum_{k\ell} b_{ij,k\ell}^* A_{k\ell}, \tag{12}$$

where $\alpha_{ij} \geq 0$, the first summation can be written in the form

$$\sum_{ij} \alpha_{ij}(A_{ij}\rho B_{ij}^\dagger + B_{ij}\rho A_{ij}^\dagger - A_{ij}^\dagger B_{ij}\rho - \rho B_{ij}^\dagger A_{ij}). \tag{13}$$

In an analogous manner we defined the operators C_{ij} by

$$\alpha_{ij}C_{ij} = \sum_{k\ell} c_{ij,k\ell} A_{k\ell}, \tag{14}$$

and the second summation becomes

$$\sum_{ij} \alpha_{ij}(A_{ij}^\dagger\rho C_{ij} + C_{ij}^\dagger\rho A_{ij} - A_{ij}C_{ij}^\dagger\rho - \rho C_{ij}A_{ij}^\dagger). \tag{15}$$

Summing up these two terms, we reach the expression

$$D = \sum_{ij} \alpha_{ij}\{[A_{ij}, \rho B_{ij}^\dagger - C_{ij}^\dagger \rho] - [A_{ij}^\dagger, B_{ij}\rho - \rho C_{ij}]\}, \qquad (16)$$

and the Lindblad equation acquires the FP structure

$$i\hbar \frac{d\rho}{dt} = [H, \rho] - \sum_{ij}\{[A_{ij}, J_{ij}^\dagger] + [A_{ij}^\dagger, J_{ij}]\}, \qquad (17)$$

where J_{ij} is given by

$$J_{ij} = i\hbar\alpha_{ij}(B_{ij}\rho - \rho C_{ij}). \qquad (18)$$

The expression (17) for the Lindblad equation is particularly meaningful because J_{ij} represents the quantum version of the probability current. Suppose that the right-hand side of (17) vanishes for a density operator ρ_0, in which case the system is said to be in a stationary state. If in addition the currents $J_{ij}(\rho_0)$ vanish, in which case $[H, \rho]$ also vanishes, then the system will be in thermodynamic equilibrium. The vanishing of the currents corresponds to the condition of detailed balance since each term of the summation in (17) vanishes. The condition of detailed balance is represented by

$$B_{ij}\rho_0 = \rho_0 C_{ij}, \qquad (19)$$

for some ρ_0.

3 Contact with Thermal Reservoirs

There are various possibilities of choosing the operators B_{ij} and C_{ij}. The only restriction is that the coefficients of the expansions (12) and (14) define Hermitian and positive matrices. The choices will depend on the type of physical conditions one wants to describe. Here we choose these operators with the purpose of describing a system in contact with several heat reservoirs at distinct temperatures. When the temperatures are all the same, then in the stationary state the system will be in thermodynamic equilibrium in which case the density operator is of the Gibbs form

$$\rho_0 = \frac{1}{Z}e^{-\beta H}, \qquad (20)$$

where β is inversely proportional to the temperature of the reservoirs.

We choose C_{ij} and B_{ij} so that

$$B_{ij}e^{-\beta_{ij}H} = e^{-\beta_{ij}H}C_{ij}, \qquad (21)$$

where β_{ij} are constants and H is the Hamiltonian. When β_{ij} has the same value, independent of i and j, the condition (21) guarantees that the detailed balance condition (19) is fulfilled and the system will be found in thermodynamic equilibrium. In other words, the system will thermalize in the long run.

A simplification arises by choosing $C_{ij} = A_{ij}$ so that B_{ij} is given by

$$B_{ij} = e^{-\beta_{ij}H}A_{ij}e^{\beta_{ij}H}, \qquad (22)$$

and the current (18) becomes

$$J_{ij} = i\hbar\alpha_{ij}(e^{-\beta_{ij}H}A_{ij}e^{\beta_{ij}H}\rho - \rho A_{ij}), \qquad (23)$$

which has the form (9) as desired.

It is now left to show that the coefficients of the expansion of B_{ij} in terms of A_{ij} are entries of a Hermitian and positive matrix. We recall that $A_{ij} = \phi_j\phi_i^\dagger$ where ϕ_i are the eigenvectors of L.

Let us denote by χ_j and E_j the eigenvectors and eigenvalues of the Hamiltonian, that is, $H\chi_i = E_i\chi_i$. The operators $X_{ij} = \chi_j\chi_i^\dagger$ can be considered a complete basis of the Liouville space. The change from this basis to the basis used above is given by the unitary transformation

$$A_{ij} = \sum_{k\ell} U_{ij,k\ell}X_{k\ell}. \qquad (24)$$

Replacing this expression in (22), we find

$$B_{ij} = \sum_{ij} U_{ij,k\ell}e^{-\beta_{ij}(E_k - E_\ell)}X_{k\ell}. \qquad (25)$$

Using

$$X_{ij} = \sum_{k\ell} U_{ij,k\ell}^\dagger A_{k\ell}, \qquad (26)$$

it can be written as

$$B_{ij} = \sum_{k\ell} G_{ij,k\ell}A_{k\ell}, \qquad (27)$$

where

$$G_{k\ell,ij}^* = \sum_{mn} U_{ij,mn}e^{-\beta_{ij}(E_m - E_n)}U_{mn,k\ell}^\dagger. \qquad (28)$$

From this expression it follows that $G_{k\ell,ij}^* = G_{ij,k\ell}$ and that the matrix with elements $G_{ij,k\ell}$ is positive, finishing our demonstration.

4 Entropy Production

The Lindblad equation or its quantum FP version (17) is supposed to describe the thermodynamic of quantum system in equilibrium or out of equilibrium. In this sense it constitutes the basic equation of a stochastic quantum thermodynamics [21, 22]. A fundamental concept in the description of systems out of thermodynamic equilibrium is the entropy production which we discuss below.

The average energy U is defined by

$$U = \text{Tr}(H\rho), \tag{29}$$

and its time evolution is obtained from the quantum FP Eq. (17), and is given by

$$\frac{dU}{dt} = \sum_{ij} \Phi_{ij}^u, \tag{30}$$

where

$$\Phi_{ij}^u = -\frac{1}{i\hbar}\{\text{Tr}[H, A_{ij}]J_{ij}^\dagger + \text{Tr}[H, A_{ij}^\dagger]J_{ij}\}, \tag{31}$$

and Φ^u is understood as the flux of energy to the system. The entropy of the system is defined by

$$S = -k\text{Tr}(\rho \ln \rho), \tag{32}$$

and its time variation is obtained from the FP Eq. (17), and is given by

$$\frac{dS}{dt} = \Pi + \Phi, \tag{33}$$

where

$$\Pi = \frac{k}{i\hbar} \sum_{ij} \text{Tr}([\ln \rho - \ln \rho_{ij}, A_{ij}]J_{ij}^\dagger) \\ + \frac{k}{i\hbar} \sum_{ij} \text{Tr}([\ln \rho - \ln \rho_{ij}, A_{ij}^\dagger]J_{ij}), \tag{34}$$

is understood as the rate of entropy production, and

$$\Phi = \frac{k}{i\hbar} \sum_{ij} \text{Tr}([\ln \rho_{ij}, A_{ij}]J_{ij}^\dagger + [\ln \rho_{ij}, A_{ij}^\dagger]J_{ij}) \tag{35}$$

is understood as the flux of entropy to the system, where ρ_{ij} is given by

$$B_{ij}\rho_{ij} = \rho_{ij}C_{ij}. \tag{36}$$

For the case of a system in contact with several heat reservoirs, $\ln \rho_{ij}$ is proportional to $-\beta_{ij}H$ and the flux of entropy can be written in the form

$$\Phi = \sum_{ij} \frac{1}{T_{ij}} \Phi_{ij}^u, \tag{37}$$

where $T_{ij} = 1/k\beta_{ij}$ and can be understood as the temperature of the heat reservoirs. We recall that Φ_{ij}^u is the energy flux, or heat flux in the present case, from each heat reservoir to the system

In the stationary state, the total flux of energy

$$\Phi^u = \sum_{ij} \Phi_{ij}^u \tag{38}$$

vanishes, but it does not mean that each flux Φ_{ij}^u vanishes because the temperatures are not all the same. In this case the flux of entropy Φ does not vanish, and $\Pi = \Phi$. As a consequence, in the nonequilibrium stationary state the production of entropy Π is nonzero. If however temperatures of the reservoirs are all the same, $T_{ij} = T$, then

$$\Phi = \frac{1}{T}\Phi^u, \tag{39}$$

and in this case Φ vanishes and so does Π, which describes a system in thermodynamic equilibrium.

5 Isolated System

Usually one describes an isolated system by the Liouville equation. This is in fact the point of depart of deriving the Lindblad equations for a given system. The given system plus the environment are assumed to be described by the Liouville equation because as a whole they are isolated, and the total energy is a conserved quantity. If the system of interest is itself isolated, then we could describe it by the Liouville equation, which means to regard the dissipative term D of Eq. (1) as nonexistent.

The mean feature of an isolated system that allows us to use the Liouville equation is that the Hamiltonian is strictly conserved along a trajectory. However, it is possible to impose a conservation of the Hamiltonian along a stochastic trajectory in such a way that the dissipation term does not need to be absent. Indeed, if we choose the operators $C_{ij} = B_{ij} = A_{ij}$ then

$$J_{ij}(\rho) = i\hbar\alpha_{ij}[A_{ij}, \rho], \tag{40}$$

and if A_{ij} commutes with the Hamiltonian $J_{ij}(H) = 0$ and the Hamiltonian will be strictly invariant.

In this case, Φ_{ij}^u vanishes identically and there will be no flux of energy, as expected. The fluxes of entropy Φ_{ij} will also vanish identically and there is no flux of entropy to or from the system. The rate of entropy production Π equals dS/dt and is given by

$$\Pi = \frac{k}{i\hbar} \sum_{ij} \text{Tr}([\ln \rho, A_{ij}]J_{ij}^\dagger + [\ln \rho, A_{ij}^\dagger]J_{ij}), \tag{41}$$

It is nonzero but vanishes in the stationary state in which case it is also the equilibrium state because J_{ij} vanishes.

6 Conclusion

We have shown that the quantum FP equation can be transformed into an equation that has the Lindblad equation. As the Lindblad equation preserves the trace and positivity of the density operator so does the quantum FP equation.

The advantage of the FP form is that one easily recognizes the quantum equivalents of the probability current and of the detailed balance condition. When the detailed balance condition is not satisfied, the quantum system in the long run will be found in a nonequilibrium stationary state. In this case the production of entropy is nonzero and can be obtained by the expression provided for the rate of entropy production. The Fokker-Planck form allows to determine a dissipation term for the case in which the Hamiltonian of the system is strictly constant, which can be understood as a closed system.

Declarations

No conflicts of interests or competing interests are related to the present work.

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