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Phenomenological criteria for the validity of quantum Markovian equations

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Abstract. We revisit the constraints on the coefficients of a quantum Markovian equation recently obtained by Dekker and Valsakumar. We extend these criteria for time-dependent coefficients and establish further criteria where appropriate phenomenological behaviour is required such as dissipation and a Boltzmann asymptotic equilibrium state.

1. Introduction

An adequate description of dissipative processes in the context of quantum mechanics is a highly nontrivial matter. The conceptual difficulties encountered are mostly related to the fact that canonical quantization is only appropriate for the description of conservative systems. One important alternative route is via the theory of dynamical semigroups, more specifically, the construction of quantum Markovian equations. This important mathematical tool has found a large number of applications in various domains of physics. However, we should point out that the matter of deriving a physically reliable master equation is complicated and delicate even for simple systems, given the many approximations and hypotheses involved. One scheme frequently adopted is to consider the system of interest coupled to a thermal reservoir taken to be sufficiently large in order to introduce the irreversible character of the equation. The dynamics of the subsystem of interest is then obtained after appropriate contraction of the reservoir's degrees of freedom is performed, in addition to the hypothesis of weak coupling and Markovian evolution. The Markovian equation so obtained takes the form

$$\frac{d}{dt}\hat{\rho}(t) = \mathcal{L}\hat{\rho}(t) \quad (1)$$

where the Liouville's superoperator \mathcal{L} is the generator of a dynamical semigroup, which can be decomposed in a Hamiltonian part (\mathcal{L}_0) and a non-Hamiltonian part (\mathcal{D}), the dissipator:

$$\mathcal{L}\hat{\rho}(t) = \frac{1}{i\hbar}[\hat{H}, \hat{\rho}(t)] + \mathcal{D}\hat{\rho}(t) \equiv (\mathcal{L}_0 + \mathcal{D})\hat{\rho}(t). \quad (2)$$

In the above equation, \hat{H} denotes a Hamiltonian operator.

It is important to remark that different approximation schemes lead to qualitatively different master equations. In this context, it is crucial to establish criteria to determine the

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validity of the approximations used [5]. From the mathematical point of view, Lindblad's structural theorem [7, 9, 10] guarantees the preservation of important general properties of the density operator, such as semidefinite positivity, during all the evolution for any initial condition. This is guaranteed if the dynamical semigroups generator has the form

$$\mathcal{L}\hat{\rho} = \frac{1}{i\hbar}[\hat{H}, \hat{\rho}] + \frac{1}{2\hbar} \sum_i ([\hat{V}_i \hat{\rho}, \hat{V}_i^\dagger] + [\hat{V}_i, \hat{\rho} \hat{V}_i^\dagger]) \quad (3)$$

where \hat{V}_i is an operator of the system of interest. Besides completely positive [7, 10], the mapping generated by the Liouvillian (3) also preserves the mixtures. These properties combined are only consistent in the case of weak coupling and hence one hopes to obtain Lindblad's form (3) in situations where this limit is verified [14, 15].

The enormous success of the rotating wave approximation (RWA) can be partly attributed to the fact that it possesses the form prescribed by the structural theorem. It is, however, easy to find counter-examples of this situation, i.e. then it can be Markovian master equations which satisfy the form of equation (3) and lead to physically unreasonable results. In what follows we use as a 'laboratory' the very well known model of an oscillator linearly coupled to a thermal bath of harmonic oscillators. In this case if we choose $\hat{V}_1 = \sqrt{2m\omega\lambda(2\bar{n}+1)}\hat{x}$ and $\hat{V}_i = 0$ for $i > 1$, a Lindblad master equation can be written as

$$\frac{d}{dt}\hat{\rho}(t) = \frac{1}{i\hbar}[\hat{H}_0, \hat{\rho}] - \frac{m\omega}{\hbar}(2\bar{n}+1)\lambda[\hat{x}, [\hat{x}, \hat{\rho}]] \quad (4)$$

where m , ω denotes the mass and frequency of the main oscillator, \bar{n} is the average number of thermal photons and λ is a constant. In the specific case of an oscillator in contact with a thermal bath, one expects the system to evolve to an equilibrium state. However, the master equation (4) describes an essentially diffusive process without incorporate dissipation. This leads to an unlimited growth in the oscillator's average energy:

$$\langle \hat{a}^\dagger \hat{a} \rangle_t = 2\lambda t(2\bar{n}+1) + \langle \hat{a}^\dagger \hat{a} \rangle_0. \quad (5)$$

It is therefore important to establish criteria, of phenomenological origin, to test the physical adequacy of the obtained master equation. Next, we shall revise and extend Dekker and Valsakumar's criteria for the preservation of the uncertainty relation and introduce the requirement that an adequate equilibrium state is asymptotically reached. In light of those criteria we analyse recent results in the literature.

2. Dekker–Valsakumar's constraints

In [6], Dekker and Valsakumar obtained the conditions to be satisfied by a master equation for the harmonic oscillator in order for the 'generalized' uncertainty

$$\sigma_{pp}\sigma_{xx} - \sigma_{px}^2 \geq \frac{1}{4}\hbar^2 \quad (6)$$

to be preserved at all times and for all initial conditions. Here, $\sigma_{pp} = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$, $\sigma_{xx} = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$, $\sigma_{px} = \frac{1}{2}(\langle \hat{p}\hat{x} + \hat{x}\hat{p} \rangle - \langle \hat{p} \rangle \langle \hat{x} \rangle)$. These conditions are expressed in terms of constraints among the diffusion and dissipation coefficients of the master equation. However, in their original work, Dekker and Valsakumar established these constraints for master equations with time-independent coefficients. As we will verify, the generalization of these criteria for master equations with time-dependent coefficients is immediate.

If the coupling between the oscillator and reservoir is linear in \hat{x} and \hat{p} , the corresponding master equation can be given generically as [9]

$$\begin{aligned} \frac{d}{dt}\hat{\rho} = \mathcal{L}\hat{\rho} = & \frac{1}{i\hbar}[\hat{H}, \hat{\rho}] - \frac{i\lambda}{2\hbar}[\hat{x}, \{\hat{\rho}, \hat{p}\}] + \frac{i\lambda}{2\hbar}[\hat{p}, \{\hat{\rho}, \hat{x}\}] - \frac{D_{pp}}{\hbar^2}[\hat{x}, [\hat{x}, \hat{\rho}]] \\ & - \frac{D_{xx}}{\hbar^2}[\hat{p}, [\hat{p}, \hat{\rho}]] + \frac{D_{px} + D_{xp}}{\hbar^2}[\hat{x}, [\hat{p}, \hat{\rho}]] \end{aligned} \quad (7)$$

where \hat{H} is chosen to be of the form

$$\hat{H} = \hat{H}_0 + \frac{\mu}{2}(\hat{p}\hat{x} + \hat{x}\hat{p}) = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 + \frac{\mu}{2}(\hat{p}\hat{x} + \hat{x}\hat{p}). \quad (8)$$

ω and \hat{H}_0 correspond, respectively, to the frequency and renormalized Hamiltonian of the oscillator to be described. The coefficients λ , D_{pp} , D_{xx} , D_{px} , D_{xp} , μ and ω can be time dependent.

Note that equation (7) can be rewritten in the form

$$\begin{aligned} \frac{d}{dt}\hat{\rho} = & \frac{1}{i\hbar}[\hat{H}_0, \hat{\rho}] - \frac{i}{2\hbar}(\lambda + \mu)[\hat{x}, \{\hat{\rho}, \hat{p}\}] + \frac{i}{2\hbar}(\lambda - \mu)[\hat{p}, \{\hat{\rho}, \hat{x}\}] \\ & - \frac{D_{pp}}{\hbar^2}[\hat{x}, [\hat{x}, \hat{\rho}]] - \frac{D_{xx}}{\hbar^2}[\hat{p}, [\hat{p}, \hat{\rho}]] + \frac{D_{px} + D_{xp}}{\hbar^2}[\hat{x}, [\hat{p}, \hat{\rho}]]. \end{aligned} \quad (9)$$

It is a simple matter to check that the master equation originally studied by Dekker and Valsakumar (equation (1) in [6]) is a particular case of equation (9) with $\lambda = \mu$.

The worst case occurs for the minimum uncertainty state

$$\sigma_{pp}\sigma_{xx} - \sigma_{px}^2 = \frac{1}{4}\hbar^2.$$

If, at a given instant, the ‘generalized’ uncertainty takes the minimum value, we shall have

$$\frac{\partial}{\partial t}(\sigma_{pp}\sigma_{xx} - \sigma_{px}^2) \geq 0 \quad (10)$$

in order to guarantee that relation (6) is satisfied for all times ($t \geq 0$). From the equation of motion for the second moments†

$$\dot{\sigma}_{pp} = -2m\omega^2\sigma_{px} - 2(\lambda + \mu)\sigma_{pp} + 2D_{pp} \quad (11a)$$

$$\dot{\sigma}_{xx} = \frac{2}{m}\sigma_{px} - 2(\lambda - \mu)\sigma_{xx} + 2D_{xx} \quad (11b)$$

$$\dot{\sigma}_{px} = -m\omega^2\sigma_{xx} + \frac{1}{m}\sigma_{pp} - 2\lambda\sigma_{px} + 2D_{px} \quad (11c)$$

we obtain

$$\begin{aligned} \frac{\partial}{\partial t}(\sigma_{pp}\sigma_{xx} - \sigma_{px}^2) = & -4\lambda \left(\sigma_{pp}\sigma_{xx} - \sigma_{px}^2 - \frac{\hbar^2}{4} \right) \\ & + 2 \left(D_{pp}\sigma_{xx} + D_{xx}\sigma_{pp} - 2D_{px}\sigma_{px} - \frac{\hbar^2\lambda}{2} \right). \end{aligned} \quad (12)$$

Taking $D_{px} = D_{xp}$ and assuming that uncertainty is minimal, we shall have

$$D_{pp}\sigma_{xx} + D_{xx}\sigma_{pp} - 2D_{px}\sigma_{px} - \frac{\hbar^2\lambda}{2} \geq 0. \quad (13)$$

† These equations of motion are easily obtained from the Wigner–Fokker–Planck equation equivalent to master equation (9).

If relation (13) is to remain valid independently of σ_{pp} , σ_{xx} and σ_{px} , the kinetic coefficients should obey the following constraints

$$D_{xx}D_{pp} - D_{px}^2 \geq \frac{\hbar^2\lambda^2}{4} \quad (14a)$$

$$D_{pp} > 0 \quad (14b)$$

$$D_{xx} > 0. \quad (14c)$$

A simple inspection of expression (13) is enough to show that inequalities (14b) and (14c) could adopt the least restrictive form $D_{pp} \geq 0$ and $D_{xx} \geq 0$. The uncertainty would still be preserved provided the kinetic coefficients satisfy (14a) and the following inequalities modified as discussed here. There are, however, two situations which are not taken into account by (14a)–(14c) in the form they were originally established. The first situation corresponds to the trivial case of unitary evolution, i.e. the dissipation and diffusion coefficients vanish. The second situation corresponds to the case where only one of diffusion coefficients, D_{pp} or D_{xx} , is zero while the other is positive. In this case, we should have $\lambda = D_{px} = 0$ so that inequality (13) is satisfied for any value of the variances σ_{pp} , σ_{xx} and σ_{px} .

2.1. The marginal case

The marginal case is characterized when the equalities $\sigma_{pp}\sigma_{xx} - \sigma_{px}^2 = \frac{1}{4}\hbar^2$ and $\frac{\partial}{\partial t}(\sigma_{pp}\sigma_{xx} - \sigma_{px}^2) = 0$ are simultaneously verified. In order to preserve the uncertainty principle, we must have

$$\frac{\partial^2}{\partial t^2}(\sigma_{pp}\sigma_{xx} - \sigma_{px}^2) \geq 0. \quad (15)$$

In this situation, the equality in equations (13) and (14a) is valid and the variances assume the special values

$$\begin{aligned} \sigma_{pp} &= \frac{D_{pp}}{\lambda} \\ \sigma_{xx} &= \frac{D_{xx}}{\lambda} \\ \sigma_{px} &= \frac{D_{px}}{\lambda}. \end{aligned} \quad (16)$$

Deriving expression (12) again, using identities (16) and equations of motion (11a)–(11c), we obtain

$$\frac{\partial^2}{\partial t^2}(\sigma_{pp}\sigma_{xx} - \sigma_{px}^2) = \frac{2}{\lambda} \frac{\partial}{\partial t} \left\{ D_{pp}D_{xx} - D_{px}^2 - \frac{\hbar^2\lambda^2}{4} \right\}. \quad (17)$$

Therefore, admitting $\lambda > 0$, in order to guarantee that uncertainty principle will not be violated in the marginal case, the inequality

$$\frac{\partial}{\partial t} \left\{ D_{pp}D_{xx} - D_{px}^2 - \frac{\hbar^2\lambda^2}{4} \right\} \geq 0 \quad (18)$$

must be verified.

Of course, the equality in equation (18) indicates the necessity to study the higher orders of time derivatives of $(\sigma_{pp}\sigma_{xx} - \sigma_{px}^2)$. Note that equation (12) yields

$$\frac{\partial^{n+1}}{\partial t^{n+1}}(\sigma_{pp}\sigma_{xx} - \sigma_{px}^2) = -4 \frac{\partial^n}{\partial t^n} \left\{ \lambda \left(\sigma_{pp}\sigma_{xx} - \sigma_{px}^2 - \frac{\hbar^2}{4} \right) \right\}$$

$$+2\frac{\partial^n}{\partial t^n} \left(D_{pp}\sigma_{xx} + D_{xx}\sigma_{pp} - 2D_{px}\sigma_{px} - \frac{\hbar^2\lambda}{2} \right) \tag{19}$$

where $n = 1, 2, \dots$. In the marginal case, if all derivatives of order equal to or less than n vanish, it will be necessary to satisfy the inequality

$$\frac{\partial^n}{\partial t^n} \left(D_{pp}\sigma_{xx} + D_{xx}\sigma_{pp} - 2D_{px}\sigma_{px} - \frac{\hbar^2\lambda}{2} \right) \geq 0 \tag{20}$$

in order to preserve the uncertainty relation.

2.2. Dekker–Valsakumar’s constraints and the structural theorem

As discussed by Săndulescu and Scutaru [9], constraints (14a)–(14c) keep an intimate connection with Lindblad’s structural theorem. If we restrict the analysis to systems linearly coupled to the thermal reservoir, the linearly independent operators to be considered are

$$\hat{V}_j = a_j \hat{p} + b_j \hat{x} \quad j = 1, 2 \tag{21}$$

where a_j and b_j ($j = 1, 2$) are complex constants. Upon substitution into equation (3) and rearranging terms so that they are in the form of master equation (9), we obtain

$$D_{pp} = \frac{\hbar}{2} \sum_{j=1}^2 |b_j|^2 \tag{22}$$

$$D_{xx} = \frac{\hbar}{2} \sum_{j=1}^2 |a_j|^2 \tag{23}$$

$$D_{px} = D_{xp} = -\frac{\hbar}{2} \text{Re} \sum_{j=1}^2 a_j^* b_j \tag{24}$$

$$\lambda = \text{Im} \sum_{j=1}^2 a_j b_j^*. \tag{25}$$

It is possible to show that constraint (14a) is verified by definitions (22)–(25) and the Schwartz inequality [8, 9]. The other constraints (14b), (14c) are only violated in cases where we have $a_1 = a_2 = 0$ and/or $b_1 = b_2 = 0$, which corresponds to the two situations we commented on above, where the uncertainty is preserved although relations (14b), (14c) are not verified. Therefore, the coefficients of a master equation of type (9) satisfies relations (14a)–(14c), if it necessarily possesses Lindblad’s canonical form.

However, some physical models and approximations yield master equations with forms different from Lindblad’s. In these cases, the positivity of the density operator is not guaranteed for all initial states (see [11–13] and section 4). Hence, it is interesting to characterize the set of initial states for which positivity is preserved for every master equation proposed. Following the ideas of Ambegaokar [11], we perform this task in the time-independent case. Consider the master equation (9) with time-independent coefficients and suppose that the initial state is $\hat{\rho}_0 = |\psi\rangle\langle\psi|$. As a result of trace conservation by equation (9), we shall impose the condition $\langle\psi|\hat{\rho}|\psi\rangle|_{t=0} \leq 0$ in order to preserve the positivity of $\hat{\rho}$. Hence,

$$\langle\psi|\dot{\hat{\rho}}|\psi\rangle|_{t=0} = \frac{i\lambda}{\hbar} \langle\hat{p}\hat{x} - \hat{x}\hat{p}\rangle_0 - \frac{2D_{pp}}{\hbar^2} \sigma_{xx}(0) - \frac{2D_{xx}}{\hbar^2} \sigma_{pp}(0) + \frac{4D_{px}}{\hbar^2} \sigma_{px}(0) \leq 0$$

yields

$$D_{pp}\sigma_{xx}(0) + D_{xx}\sigma_{pp}(0) - 2D_{px}\sigma_{px}(0) - \frac{\hbar^2\lambda}{2} \geq 0. \quad (26)$$

The set of initial statistical operators that preserve the positivity is characterized by the class of states for which the second moments $\sigma_{xx}(0)$, $\sigma_{pp}(0)$ and $\sigma_{px}(0)$ verify the inequality (26). This inequality is equivalent to the fundamental inequality (13) with time-independent coefficients, therefore the initial states which preserve the positivity also preserve the ‘generalized’ uncertainty principle (6).

3. Stationarity of the Gibbs equilibrium state

3.1. The time-independent case

If the kinetic coefficients in equation (9) are constants, one may expect some tendency to equilibrium to occur. In the particular case of equation (4), the equilibrium state does not exist since this equation describes a purely diffusive process. Equation (4) illustrates one of two situations previously mentioned in section 2 for which constraints (14b) and/or (14c) are violated but the uncertainty principle is still preserved. Actually, the diffusion coefficient D_{pp} is positive while the other coefficients vanish.

Dissipation and diffusion are fundamental processes in what concerns the dynamics of a quantum system coupled to the thermal bath and one cannot exist without the other, if physically consistent results are required. In fact, if dissipation is eliminated ($\lambda = 0$) the reservoir fluctuating forces will transfer energies into the system in an unlimited way. On the other hand, if we eliminated diffusion ((14a), (14b) or (14c) not satisfied) the system can eventually occupy a volume in phase space which is forbidden by the uncertainty principle and violate it [8, 9].

3.2. Conditions for stationarity of the Gibbs state

We now proceed to investigate whether the constraints just derived are enough to guarantee that the system will reach an asymptotic equilibrium (Gibbs) state of the form

$$\hat{\rho}^{eq} = \frac{e^{-\beta\hat{H}_0}}{\text{tr} e^{-\beta\hat{H}_0}} \quad (27)$$

where $\beta = \frac{1}{k_B T}$, k_B denotes the Boltzmann constant, T is the reservoir temperature and \hat{H}_0 is the renormalized Hamiltonian of the system. Considering this state, the master equation (9) and imposing the equilibrium condition

$$\mathcal{L}\hat{\rho}^{eq} = 0 \quad (28)$$

we obtain

$$D_{px} = -D_{xp} \quad (29)$$

$$D_{pp} = \frac{m\hbar\omega}{2}(2\bar{n} + 1)(\lambda + \mu) \quad (30)$$

$$D_{xx} = \frac{\hbar}{2m\omega}(2\bar{n} + 1)(\lambda - \mu). \quad (31)$$

Expressions (29)–(31) establish the relations that the kinetic coefficients and parameters μ and ω must satisfy so that the state given in (27) is an equilibrium state of the master equation in question. These relations are strict correspondence with equalities (5.4) of [8].

Combining equations (30) and (31) with inequalities (14b) and (14c) and considering $\lambda > 0$ we obtain a restriction on the friction coefficient so that the master equation (9) verifies both the stationarity condition and the uncertainty condition:

$$\lambda > |\mu|.$$

On the other hand, if we combine relations (29)–(31) with inequality (14a) we can determine the minimum value for the dissipation coefficient:

$$\lambda_{\min} = \frac{|\mu|}{\sqrt{1 - \frac{1}{(2\bar{n}+1)^2}}}. \quad (32)$$

This relation determines the minimum value that the dissipation coefficient can have in order for the solution to preserve the uncertainty relation and furthermore reach the appropriate stationary state asymptotically. It is interesting to note that, for example, the master equation originally studied by Dekker and Valsakumar cannot simultaneously verify the stationary condition and preserve the generalized uncertainty for any finite temperature. As discussed by Lindblad [8], the equations of motion for the observables of the system of interest generated by a master equation of the type (9) maintain a close analogy to those of the classical Brownian motion if the condition $\lambda = \mu$ is verified. However, relation (32) shows that, in this case, the equipartition and structural theorem are only compatible in the limit $T \rightarrow \infty$.

4. An application: limits of validity for the non-RWA master equation

Despite the success obtained by the RWA master equation, its application is limited to those systems where the ratio between the dissipation coefficient and the natural frequency is $\frac{\lambda}{\omega} \ll 1$. In quantum optics, this situation occurs when systems with largely spaced energy levels are weakly coupled to the set of modes of the electromagnetic field. However, if we regard systems which are strongly damped, with quasidegenerate or closely spaced energy levels, the use of the RWA master equation becomes inadequate, since it can yield incorrect results [13].

There are several methods which do not employ the RWA [1–4]. They independently lead to the following master equation for a Brownian particle coupled to a thermal reservoir at temperature T

$$\frac{d}{dt} \hat{\rho} = -\frac{i}{\hbar} [\hat{H}_0, \hat{\rho}] - \frac{i\lambda}{\hbar} [\hat{x}, \{\hat{\rho}, \hat{p}\}] - \frac{2m\lambda}{\beta\hbar^2} [\hat{x}, [\hat{x}, \hat{\rho}]]. \quad (33)$$

This expression is a particular form of the master equation (9) with $\mu = \lambda$, $D_{pp} = \frac{2m\lambda}{\beta}$ and $D_{px} = D_{xp} = D_{xx} = 0$, in the limit of high enough temperatures. Munro and Gardiner [13] baptized this equation the ‘non-rotating-wave (NRW) master equation’.

The first important thing to be noticed about the NRW master equation is that it does not possess Lindblad’s structural form. This means, in particular, that the density operator obtained from it will not preserve the semidefinite positivity condition for a certain class of initial states (see [11–13] and references therein). Substituting the coefficients of equation (33) into inequality (26), we obtain the following restriction on the initial states to be observed in the NRW master equation

$$\sigma_{xx} \geq \frac{\beta\hbar^2}{4m}. \quad (34)$$

Since σ_{xx} represents the uncertainty in position inequality (34) determines the minimum value of dispersion that the variable \hat{x} should have in order for the positivity (and the 'generalized' uncertainty principle) to be preserved in time.

Although the anomalous behaviour of the NRW master equation is present even in the case of the harmonic oscillator, it is interesting to note that equation (33) satisfies the stationarity condition, since relations (29)–(31) are verified. This anomalous behaviour of the NRW equation has led some authors to propose modifications in the equation to remove the problem. Among the proposed modifications, we discuss the one which suggests the addition of new terms to the original equation in order to cast it into Lindblad's form [12, 11]. A term of type

$$-\frac{\kappa\lambda\beta}{8m}[\hat{p}, [\hat{p}, \hat{\rho}]]$$

is added to equation (33). If $\kappa > 1$, this new term will bring the equation into the form of the structural theorem, thus saving the positivity and the uncertainty principle. There is, however, a consequence of the *ad hoc* inclusion of this term: the appropriate equilibrium (Gibbs) state (27) leaves to be the asymptotic state.

5. Conclusion

In this work, we have discussed the importance of the phenomenological criteria in the study of Markovian master equations. Using the harmonic oscillator as a 'laboratory', we explored two of these criteria. The first criterion refers to Dekker–Valsakumar's constraints [6], which establish the relations among the kinetic coefficients of a master equation in order to preserve the uncertainty principle. We extended this criterion for master equations with time-dependent coefficients.

Dekker–Valsakumar's constraints are closely related to Lindblad's structural theorem [9], also the preservation of positivity is related to the preservation of 'generalized' uncertainty. This relation was illustrated in the particular case of the NRW master equation. Actually, the set of initial states which preserve the positivity of the density operator and the uncertainty principle is subject to the same restriction.

The second criteria refers to the stationarity of the equilibrium state. We established the relations that the kinetic coefficients must satisfy in order for the Gibbs state (27) to be stationary. As an example of applications, we verified that the modification proposed by some authors [12, 11] in order for the NRW master equation to take the Lindblad's form leads to the violation of the stationarity of the Gibbs equilibrium state.

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