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Quantum dissipation and phenomenological approaches*

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Using Terwiel's cumulants the Markovian approximation to arrive to the Quantum Master Equation, for a system interacting with a thermal bath, is revisited. The second order weak coupling approximation is analyzed, then a Kossakowski-Lindblad form for the generator is written in terms of the position and momentum operators. A weak coupling approximation for the stochastic non-Markovian wave function is worked out. A free particle model interacting with a thermal quantum bath is studied in the context of Schrödinger-Langevin picture. A phenomenological point of view is introduced in order to overcome certain difficulties in the time evolution – in the second order approximation – for the free particle Hamiltonian.

Key words: *quantum open systems, quantum master equation, stochastic Schrödinger equations*

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1. Introduction

In nature many quantum systems behave like open dissipative *bodies* when their dynamical variables are coupled to the infinite degrees of freedom of the surrounding. The interaction between the open system $\mathcal{S}$ and its environment often leads to dissipation, fluctuation, decoherence and irreversible processes. The description of the dynamics of $\mathcal{S}$ has historically been based on the analysis of the reduced density matrix, ρ, formalism, within which both the *intrinsic quantum fluctuations* of $\mathcal{S}$ and the *quantum noise*, due to the environment, can be incorporated in a unified manner. The general evolution equation for ρ is derived from the *unitary* Hamil-

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tonian dynamics of the whole corresponding universe. Then, eliminating the bath variables, a reduced dynamics can be introduced by an *effective* evolution equation of the form:

$$\dot{\rho}\,(t) = L[\rho\,(t)]$$

This expression is in analogy with a *classical* transport dynamics, which determines the evolution of any open system $\mathcal{S}$.

In the Markovian framework Kossakoswki [1] and Lindblad [2] have established the *structure* of the master equation (the semigroup generator) in order that the dynamics of the quantum system be well behaved. In this way the semigroup is a completely positive map and preserves trace, positivity, and hermiticity of ρ during all its time evolution. A completely positive semigroup is characterized by the generator

$$L\,[\bullet] \equiv -\frac{\mathrm{i}}{\hbar}[H_{\mathrm{eff}}, \bullet] + \frac{1}{2\hbar}\sum_{\alpha}\left[V_\alpha \bullet, V_\alpha^\dagger\right] + \left[V_\alpha, \bullet V_\alpha^\dagger\right], \tag{1.1}$$

where V_α is any bounded operator of $\mathcal{S}$; this generator can also be written in a different way. Taking into account an operator basis $\{S_\alpha\}$ of the $N \times N$ complex matrices, the alternative expression is given in terms of the superoperator $F[\bullet] = (1/2\hbar)\sum_{\alpha,\gamma} a_{\alpha\gamma} S_\alpha \bullet S_\gamma^\dagger$, $\alpha, \gamma = 1, ..., N^2 - 1$ and its dual[3] $F^*[\bullet]$, then (1.1) is rewritten as

$$L\,[\bullet] = -\frac{\mathrm{i}}{\hbar}[H_{\mathrm{eff}}, \bullet] + F[\bullet] - \frac{1}{2}\,\{F^*[I], \bullet\}_+ \ , \tag{1.2}$$

where I is the identity operator and $[a_{\alpha\gamma}]$ is positive definite (*structural theorem* [2]).

In general we call an expression like (1.2) a Kossakowski-Lindblad (KL) *form* [3]. The map will be a completely positive semigroup if and only if the hermitian matrix $[a_{\alpha\gamma}]$ is positive definite [1,4,5]. If the generator is written as in (1.2) with a non-positive matrix $[a_{\alpha\gamma}]$, we say that the KL *form* does not satisfy the structural theorem.

Starting from a microscopic dynamics (a system $\mathcal{S}$ coupled to some reservoir $\mathcal{B}$) the Quantum Master Equation (QME) has been derived in several different ways [4–6]. One of these derivations comes from a perturbative *ordered expansion*, which can be obtained by *tracing-out* the bath variables. If any evolution time of the system is much greater than the correlation time of the bath, and a separable structure for the density matrix is assumed, a Markovian dominant contribution can be found. Hence in a second order approximation (in the coupling parameter) the QME has a KL *form,* but in general, it is not completely positive [3]. For systems with discrete levels of energy and in the weak coupling approximation, it is always possible to introduce an average formalism that leads to a bonafide KL generator. This general procedure is the Davies device [7]; in the context of quantum optics there is an equivalent approach known as the Rotating Wave Approximation (RWA) [8]. The dynamics of an open system can alternatively be understood through the use of stochastic equations for the state vector of $\mathcal{S}$. This point of view includes the (linear and non-linear) quantum state diffusion approach [9], the wave packet reduction

[3]Defined by $\mathrm{Tr}(F^*[A]\rho) = \mathrm{Tr}(AF[\rho])$.

[10,11] and the quantum jump processes [12]. The Shrödinger-Langevin (SL) picture [3,6,13] belongs to this formulation and its interest resides in giving an alternative way to obtain the QME with a KL *form*. This fact has allowed us to define a *mapping* between the SL and the *tracing-out* technique, therefore establishing a non-Markovian dynamics for the open system $\mathcal{S}$ that can reproduce (in the Markovian limit) the behaviour of the QME obtained from tracing-out the bath variables. This kind of stochastic formalism has the additional advantage that can be applied to very different environments, then the influence of the quantum bath can be taking into account by using arbitrary random operators in the SL equation.

The path integral method is another formalism for eliminating the bath variables, which starts from the total Hamiltonian of the system $\mathcal{S}$ plus $\mathcal{B}$ [14]. We note that in general the kind of interactions and environments (infinite set harmonic oscillators) treated by the path integral formalisms give rise to a Gaussian influence functional. One of the pioneer work belongs to Caldeira and Leggett [15] who obtained the QME in the high temperatures limit by using some Ohmic linear coupling between $\mathcal{S}$ and $\mathcal{B}$. With these assumptions Caldeira and Leggett's QME has a kernel local in time. Other types of coupling with the environment can also be assumed [16,17].

It is important to remark that in general a Markovian approximation does not satisfy the structural theorem, i.e. does not generate completely positive semigroups (this fact can lead to non-positive or to non-physical density matrices during the early short-time evolution [6,18]). Then many different approximations have been introduced to overcome this difficulty. For example in the context of the weak coupling approximation we could introduce some restrictions to the interaction Hamiltonian, in order to fulfil a necessary condition for the completely positivity character [3]. Recently a path integral approach at intermediate temperatures has been considered [19], therefore obtaining a bonafide KL. Also a pure phenomenological description can be useful to build quantum dissipative semigroups. This approach consists in considering, *ad-hoc,* suitable interaction operators V_α in the generator (1.1) [20,21]. In this case the generator does not have any problem of positivity, but it is necessary to *postulate* a suitable temperature dependence in V_α, so that the evolution leads to the corresponding thermal equilibrium state of $\mathcal{S}$.

In this work we are concerned with those mentioned formalisms by giving a revision to the Markovian and weak coupling approximation; in addition we are going to apply the SL picture to the free particle model. This paper is organized as follows. In section 2 we present the general approach, using Terwiel's cumulants, to derive a perturbative QME from the total microscopic Hamiltonian. In section 3 we are concerned with the second order approximation: first we review the results from tracing-out; second in the context of the SL picture we give a *mapping* with the trace-out technique. In section 4 we analyze the second order QME written in terms of p, q the momentum and position operators respectively. In section 5 we show some results concerning the free particle Hamiltonian in interaction with a thermal bath; in the same section we also give a phenomenological treatment to overcome some difficulties in the evolution of the free particle model. In section 6 we present some conclusions concerning our results. Some mathematical details about the Terwiel cumulants, the correlation functions and the completely positive condition can be found in the appendixes.

2. Tracing-out the bath and the Markovian approximation

The tracing out technique starts from the total Hamiltonian $H_{\mathrm{T}} = H_{\mathrm{S}} + H_{\mathrm{B}} + \theta H_{\mathrm{I}}$ where the first two terms correspond to system and bath Hamiltonians and θH_{I} is the interaction contribution being θ the coupling strength. The Liouville equation for the total density matrix ρ_{T} is written in terms of the Liouvillian superoperator $\mathcal{L}[\bullet] = -\mathrm{i}/\hbar[H, \bullet]$, then the evolution for the total (closed) system is

$$\dot{\rho}_{\mathrm{T}} = (\mathcal{L}_0 + \theta\mathcal{L}_{\mathrm{I}})\rho_{\mathrm{T}} \ . \tag{2.1}$$

Without any interaction the system evolves with the Hamiltonian $H_0 = H_{\mathrm{S}} + H_{\mathrm{B}}$. To obtain an equation for the reduced density matrix, $\rho = \mathrm{Tr}_{\mathrm{B}}(\rho_{\mathrm{T}})$, we *trace-out* the bath variables assuming a factorized initial condition $\rho_{\mathrm{T}}(0) = \rho(0) \otimes \rho_{\mathrm{B}}$, where ρ_{B} denotes the bath equilibrium statistical operator. In the interaction representation $\sigma_{\mathrm{T}}(t) = \exp(-\mathcal{L}_0 t)\rho_{\mathrm{T}}(t)$ where $\mathcal{L}_{\mathrm{I}}(t) = \exp(-\mathcal{L}_0 t)\mathcal{L}_{\mathrm{I}} \exp(\mathcal{L}_0 t)$, the unitary evolution equation is

$$\dot{\sigma}_{\mathrm{T}}(t) = \theta\mathcal{L}_{\mathrm{I}}(t)\sigma_{\mathrm{T}}(t). \tag{2.2}$$

This equation can formally be integrated

$$\sigma_{\mathrm{T}}(t) = \hat{T}\exp\left(\theta\int_0^t \mathcal{L}_{\mathrm{I}}(t_1)\mathrm{d}t_1\right)\sigma_{\mathrm{T}}(0), \tag{2.3}$$

where $\hat{T}$ denotes the time ordering operator. Tracing-out the bath variables gives

$$\sigma(t) = \mathrm{Tr}_{\mathrm{B}}[\sigma_{\mathrm{T}}(t)] = \left\langle \hat{T}\exp\left(\theta\int_0^t \mathcal{L}_{\mathrm{I}}(t_1)\mathrm{d}t_1\right)\right\rangle_{\mathrm{B}} \sigma(0), \tag{2.4}$$

where we have denoted $\langle\bullet\rangle_{\mathrm{B}} = \mathrm{Tr}_{\mathrm{B}}\,[\bullet\rho_{\mathrm{B}}]$. Under this average expectation $\mathcal{L}_{\mathrm{I}}(t)$ behaves like a stochastic superoperator with zero mean $\langle\mathcal{L}_{\mathrm{I}}(t_1)\rangle_{\mathrm{B}} = 0$, which is the case in the most applications. The average and the time ordering commute, then we can expand the exponent in cumulants [6]

$$\sigma(t) = \hat{T}\exp\left(\int_0^t \mathrm{d}t_1 \int_0^{t_1} \theta^2 \left\langle\left\langle\mathcal{L}_{\mathrm{I}}(t_1)\mathcal{L}_{\mathrm{I}}(t_2)\right\rangle\right\rangle_{\mathrm{B}}\ \mathrm{d}t_2 + \cdots\right)\sigma(0). \tag{2.5}$$

Nevertheless in (2.5) we still have the time ordering operator telling that after expanding the different terms of the exponential the individual factors inside the integrands must be ordered with the smaller times at the right. Assuming that the correlation function of the bath has a well defined correlation time τ_{c}, an ordered expansion in terms of Kubo's number $\mathcal{O}(\theta^2\tau_{\mathrm{c}})$ can be performed in the argument of the exponential (2.5) [22], see appendix A

$$\sigma(t) = \hat{T}\exp\left(\int_0^t \sum_{n=2}^{\infty} \theta^n K_n(t')\mathrm{d}t'\right)\sigma(0), \tag{2.6}$$

where

$$K_n(t) = \int_0^t \mathrm{d}t_1 \cdots \int_0^{t_{n-2}} \mathrm{d}t_{n-1} \left\langle \mathcal{L}_\mathrm{I}(t)\mathcal{L}_\mathrm{I}(t_1)\cdots\mathcal{L}_\mathrm{I}(t_{n-1})\right\rangle_\mathrm{B}^p \, , \tag{2.7}$$

here $\langle A(t)\cdots A(t_{n-1})\rangle_\mathrm{B}^p$ is the *ordered* cumulant as defined in [6,22,23]. This ordered cumulants have a "cluster" property telling us that the cumulant vanish whenever two successive times fulfil $|t_i - t_{i+1}| \geqslant \tau_\mathrm{c}$. This fact allows us to write a Markovian equation for the dynamics of the system $\mathcal{S}$ considering $t \gg \tau_\mathrm{c}$. Going back to the original representation the result is

$$\dot{\rho}(t) = \left(\mathcal{L}_\mathrm{S} + \sum_{n=2}^{\infty} \theta^n \exp(\mathcal{L}_\mathrm{S} t) K_n(\infty) \exp(-\mathcal{L}_\mathrm{S} t)\right)\rho(t). \tag{2.8}$$

The well known second order Markovian approximation (weak coupling limit) reads

$$\dot{\rho}(t) = \mathcal{L}_\mathrm{S}\rho(t) - \frac{\theta^2}{\hbar^2}\int_0^\infty \mathrm{d}\tau\, \mathrm{Tr}_\mathrm{B}\left([H_\mathrm{I}, [H_\mathrm{I}(-\tau), \rho_\mathrm{B}^\mathrm{e}\otimes\rho(t)]]\right) + \mathcal{O}(\theta^3\tau_\mathrm{c}^2), \tag{2.9}$$

where $H_\mathrm{I}(-\tau)$ is the Heisenberg evolution of H_I under the free Hamiltonian H_0. This is the Markovian approximation for any arbitrary open system $\mathcal{S}$ interacting with a bath.

Now let us analyze a particular bath $\mathcal{B}$ and interaction H_I. Here we assume that $\mathcal{B}$ is composed by an infinite set of harmonic oscillators so $H_\mathrm{B} = \sum_k \hbar\omega_k b_k^\dagger b_k$ and $b_k^\dagger, b_k$ create and annihilate bosons of frequency ω_k. The interaction Hamiltonian is taken as $H_\mathrm{I} = B\otimes V$ with the bath operator $B = \sum_k v_k(b_k^\dagger + b_k)$ where v_k are the coupling constants. It can be proved that the bath operator (in the Heisenberg representation) $B(t)$ behaves like a Gaussian stochastic process (under the average $\mathrm{Tr}[\rho_\mathrm{B}\bullet]$) with a non-white correlation [24]

$$\chi(-\tau) = \left\langle B^\dagger B(-\tau)\right\rangle_\mathrm{B} = \sum_k |v_k|^2[\exp(\mathrm{i}\omega_k\tau)n(\omega_k) + \exp(-\mathrm{i}\omega_k\tau)(n(\omega_k)+1)] \, , \tag{2.10}$$

here $n(\omega_k)$ is the phonon number at frequency ω_k. In this case the statistical properties of $\mathcal{L}_\mathrm{I}(t)$ will be characterized by Gaussian processes. Therefore the exponent (2.5) will only involve a second order cumulant, hence it can be written in the familiar form [14,15]

$$\begin{aligned}\sigma(t) \;=\; & \hat{T}\exp\Big[-(\theta^2/\hbar^2)\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \left(V_+(t_1) - V_-(t_1)\right) \\ & \times \left(\chi(t_2 - t_1)V_+(t_2) - \chi^*(t_2 - t_1)V_-(t_2)\right)\Big]\sigma(0).\end{aligned} \tag{2.11}$$

Note that (2.11) is written in the interaction representation, and we have used the notation $V_+[\bullet] = V\bullet$ and $V_-[\bullet] = \bullet V$. We remark that this expression is exact because of the Gaussian statistic and the linear interaction H_I between $\mathcal{S}$ and $\mathcal{B}$.

In the context of a path integral formalism the propagator (2.11) is also obtained as the result of working with a bosonic bath and a linear coupling, therefore leading to a Gaussian influence functional [14,15,19]. Note that in the case of a Gaussian statistics (for the Liouvillian $\mathcal{L}_{\rm I}(t)$) the second order dominant contribution (2.9) is only an approximation. This happens because for a Gaussian statistics the normal cumulants in (2.5) vanish for the order greater than two, but we still have to work out the *ordered* cumulants in the integrand of K_n (for $n > 2$) in (2.7). This is so because of the non-commuting character of $V(t)$ at different times.

Now let us review, in this context, the Caldeira and Leggett assumptions. They assume Ohmic coupling $|v_k|^2 \sim g\omega_k$ when $\omega_k \leqslant \Omega_{\rm C}$, high bath temperature, and high frequency cut-off $\Omega_{\rm C}$. Then the complex correlation (2.10) becomes $\chi_\infty(-\tau) = (2\pi g/\beta\hbar)\tilde{\delta}(\tau) + {\rm i}g\pi\tilde{\delta}'(\tau)$. Here β is proportional to the inverse temperature and the function $\tilde{\delta}(\tau) = \frac{1}{\pi}\int_0^{\Omega_{\rm C}} \cos(\omega\tau){\rm d}\omega$ turns out to be a Dirac-delta in the limit $\Omega_{\rm C} \to \infty$. In this case the correlation time vanishes and the second order approximation (2.9) becomes exact. Taking $\gamma = g\pi/\hbar$ and $\theta = 1$ we get for the QME [15,25]

$$\dot{\rho}(t) = \frac{-{\rm i}}{\hbar}[H_{\rm S} - \gamma\tilde{\delta}(0)V^2, \rho(t)] - \frac{\gamma}{\hbar^2\beta}\,[V, [V, \rho(t)]] + \frac{\gamma}{2\hbar^2}\left[V, [[H_{\rm S}, V]\,, \rho(t)]_+\right]. \quad (2.12)$$

This result is exact because if $\tau_{\rm c} = 0$ the “cluster” property leads to the fact that any *ordered* cumulant vanishes for $n > 2$. Equation (2.12) is a generalization of Caldeira & Leggett's QME [15], in that paper they only worked the case $V = q$, being q the coordinate operator of the system $\mathcal{S}$.

3. The second order approximation revisited

3.1. Tracing-out the bath variables

In this section we will review the form that the second order Markovian approximation (2.9) takes. This second order QME [4–6,8,25] has the KL *form* (1.2); the effective Hamiltonian $H_{\rm eff}$ and fluctuation superoperator $F[\bullet]$ are [3]:

$$H_{\rm eff} = H_{\rm S} - {\rm i}\frac{\theta^2}{2\hbar}\int_0^\infty {\rm d}\tau\, {\rm Tr}_{\rm B}\left([H_{\rm I}, H_{\rm I}(-\tau)]\,\rho_{\rm B}^{\rm e}\right), \quad (3.1)$$

$$F[\rho(t)] = \left(\frac{\theta}{\hbar}\right)^2\int_0^\infty {\rm d}\tau\, {\rm Tr}_{\rm B}\left(H_{\rm I}\;\rho(t)\otimes\rho_{\rm B}^{\rm e}\; H_{\rm I}(-\tau) + H_{\rm I}(-\tau)\,\rho(t)\otimes\rho_{\rm B}^{\rm e}\, H_{\rm I}\right). \quad (3.2)$$

Taking $H_{\rm I} = \sum\limits_\alpha V_\alpha \otimes B_\alpha$ (in terms of system operators V_α and bath operators B_α) the correlation functions of the bath read:

$$\chi_{\alpha\beta}(-\tau) \equiv {\rm Tr}_{\rm B}\left(\rho_{\rm B}^{\rm e}\; B_\alpha^\dagger\, B_\beta(-\tau)\right), \quad (3.3)$$

so equations (3.1) and (3.2) can be rewritten in the form

$$H_{\rm eff} = H_{\rm S} - {\rm i}\frac{\theta^2}{2\hbar}\sum_{\alpha\beta}\int_0^\infty {\rm d}\tau\,\Big(\chi_{\alpha\beta}(-\tau)V_\alpha^\dagger V_\beta(-\tau) - \chi_{\alpha\beta}^*(-\tau)V_\beta^\dagger(-\tau)V_\alpha\Big), \quad (3.4)$$

$$F[\bullet] = \left(\frac{\theta}{\hbar}\right)^2\sum_{\alpha\beta}\int_0^\infty {\rm d}\tau\,\Big(\chi_{\alpha\beta}(-\tau)V_\beta(-\tau)\bullet V_\alpha^\dagger + \chi_{\alpha\beta}^*(-\tau)V_\alpha\bullet V_\beta^\dagger(-\tau)\Big). \quad (3.5)$$

Now let us define the auxiliary correlation function

$$\Gamma_{\alpha\beta}(-\tau) \equiv \mathrm{Tr_B}\left(\rho_{\mathrm{B}}^{\mathrm{e}}\ B_\alpha\, B_\beta(-\tau)\right).$$

Then note that because H_{I} is hermitian, there always exists a α' such that $V_\alpha^\dagger = V_{\alpha'}$ and $B_\alpha^\dagger = B_{\alpha'}$, so $\Gamma_{\alpha'\beta}(-\tau) = \chi_{\alpha\beta}(-\tau)$ (thus indicating that $\Gamma_{\alpha\beta}$ is only a change in the notation). This fact allows us to write the effective Hamiltonian in terms of $\Gamma_{\alpha\beta}(-\tau)$ in the form

$$H_{\mathrm{eff}} = H_{\mathrm{S}} - \mathrm{i}\frac{\theta^2}{2\hbar}\sum_{\alpha\beta}\int_0^\infty \mathrm{d}\tau\left(\Gamma_{\alpha\beta}(-\tau)V_\alpha V_\beta(-\tau) - \Gamma^*_{\alpha\beta}(-\tau)V_\beta^\dagger(-\tau)V_\alpha^\dagger\right). \qquad (3.6)$$

From equation (3.2) it is possible to see that the second order QME coming from trace-out technique is not, in general, completely positive. In a previous work we established some restrictions on H_{I} in order to arrive to a bonafide KL [3].

3.2. The Shrödinger-Langevin approach

The starting point in the Shrödinger-Langevin (SL) approach is a phenomenological equation for the *stochastic wave function* of the open system $\mathcal{S}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left|\Psi\right\rangle = \left[\frac{-\mathrm{i}}{\hbar}H_{\mathrm{S}} - \frac{\theta}{\hbar}\left(U + \mathrm{i}\,\mathcal{F}\left(t\right)\right)\right]\left|\Psi\right\rangle, \qquad (3.7)$$

where $U \equiv U_{\mathrm{R}} + \mathrm{i}U_{\mathrm{I}}$ ($U_{\mathrm{R}}, U_{\mathrm{I}}$ are hermitian operators) is a deterministic operator to be found later on, and $\mathcal{F}\left(t\right)$ is an arbitrary mean value zero stationary stochastic operator; here we have made evident the $\hbar$. The reduced density matrix, for the system $\mathcal{S}$, is defined as the average of the external product of the wave function $\rho = \left\langle|\Psi\rangle\langle\Psi|\right\rangle_{\mathcal{F}\mathcal{F}^\dagger}$. Hence performing a cumulant expansion in $\mathcal{O}(\theta^m\tau_{\mathrm{c}}^{m-1})$ where τ_{c} is the correlation time of the random operator $\mathcal{F}\left(t\right)$, and considering $t \gg \tau_{\mathrm{c}}$ the second order contribution has, once again, the KL *form* (1.2). The operator U is obtained, consistently, in order to preserve the trace $\mathrm{Tr}[\rho] = 1$ during all the evolution of $\rho(t)$

$$U + U^\dagger = 2U_{\mathrm{R}} = \frac{\theta}{\hbar}\int_0^\infty \mathrm{d}\tau\left(\left[\left\langle\left\langle\mathcal{F}^\dagger\left(t\right)\mathcal{F}\left(t-\tau\right)\right\rangle\right\rangle - \left\langle\left\langle\mathcal{F}\left(t\right)\mathcal{F}\left(t-\tau\right)\right\rangle\right\rangle\right] + \mathrm{h.c.}\right). \qquad (3.8)$$

Note that the last condition only fix the hermitian part of U. Considering (3.8) the terms in the KL *form,* in the context of the SL picture, are characterized by

$$H_{\mathrm{eff}} = H_{\mathrm{S}} + \theta U_{\mathrm{I}} - \mathrm{i}\frac{\theta^2}{2\hbar}\int_0^\infty \mathrm{d}\tau\left(\left\langle\left\langle\mathcal{F}\left(t\right)\mathcal{F}\left(t-\tau\right)\right\rangle\right\rangle - \left\langle\left\langle\mathcal{F}^\dagger\left(t-\tau\right)\mathcal{F}^\dagger\left(t\right)\right\rangle\right\rangle\right), \qquad (3.9)$$

$$F\left[\bullet\right] = \frac{\theta^2}{\hbar^2}\int_0^\infty \mathrm{d}\tau\left(\left\langle\left\langle\mathcal{F}\left(t\right)\bullet\mathcal{F}^\dagger\left(t-\tau\right)\right\rangle\right\rangle + \left\langle\left\langle\mathcal{F}\left(t-\tau\right)\bullet\mathcal{F}^\dagger\left(t\right)\right\rangle\right\rangle\right). \qquad (3.10)$$

Note that there is a freedom in the arbitrary selection of U_{I}, this fact can be used to obtain a desired H_{eff}. We can distinguish two possibilities: (i) hermitian U (so

$U_{\mathrm{I}}=0$) then equation (3.9) shows that the effective Hamiltonian depends only on the correlations $\langle\langle\mathcal{F}(t)\,\mathcal{F}(t-\tau)\rangle\rangle$ and in contrast $F[\bullet]$ depends on $\left\langle\left\langle\mathcal{F}(t-\tau)\,\mathcal{F}^{\dagger}(t)\right\rangle\right\rangle$ [3]; (ii) non-hermitian U (so $U_{\mathrm{I}}\neq 0$) then from (3.8) we can choose U in the particular form

$$U=\frac{\theta}{\hbar}\int_{0}^{\infty}\mathrm{d}\tau\left(\left\langle\left\langle\mathcal{F}^{\dagger}(t)\,\mathcal{F}(t-\tau)\right\rangle\right\rangle-\left\langle\left\langle\mathcal{F}(t)\,\mathcal{F}(t-\tau)\right\rangle\right\rangle\right). \tag{3.11}$$

Therefore the effective Hamiltonian becomes

$$H_{\mathrm{eff}}=H_{\mathrm{S}}-\mathrm{i}\frac{\theta^{2}}{2\hbar}\int_{0}^{\infty}\mathrm{d}\tau\left(\left\langle\left\langle\mathcal{F}^{\dagger}(t)\,\mathcal{F}(t-\tau)\right\rangle\right\rangle-\left\langle\left\langle\mathcal{F}^{\dagger}(t-\tau)\,\mathcal{F}(t)\right\rangle\right\rangle\right), \tag{3.12}$$

so for the case of a non-hermitian U, all the contributions into the KL *form* can be written just in terms of $\left\langle\left\langle\mathcal{F}^{\dagger}(t-\tau)\,\mathcal{F}(t)\right\rangle\right\rangle$. As we have pointed out in the introduction this second order approximation, in general, and for any operator $\mathcal{F}(t)$, is not completely positive. Hence some restrictions ought to be given in order to guarantee a bonafide KL [3].

From now on we choose for the random operator $\mathcal{F}(t)$ in (3.7) the particular form

$$\mathcal{F}(t)=\sum_{\alpha}l_{\alpha}(t)V_{\alpha} \tag{3.13}$$

where $l_{\alpha}(t)$ are complex-value c-noises. Then from (3.10) $F[\bullet]$ is *formally* equivalent to (3.5) replacing $\chi_{\alpha\beta}(-\tau)$ by $\langle\langle l_{\alpha}^{*}(t)\; l_{\beta}(t-\tau)\rangle\rangle$. The SL formalism allows us to analyze any arbitrary correlation functions that could mimic different environments. In this way we arrive to a linear evolution equation for the *stochastic wave function*, hence representing a diversity of dynamics for the open system of interest [3].

One of the situations that we want to mimic, by using the SL picture, is the corresponding reduced dynamics obtained in the *tracing-out* context, equations (3.1) and (3.2). We note that this comparison can be done only in the case when $\mathcal{F}(t)$ is non-hermitian. Identifying the noise correlations with those that come from the quantum bath a *numeric* equivalence is obtained with all the terms in the KL *form*. The mapping for these correlations is:

$$\langle\langle l_{\alpha}^{*}(t)\; l_{\beta}(t-\tau)\rangle\rangle\equiv\chi_{\alpha\beta}(-\tau), \tag{3.14}$$

and consistently chosen

$$\langle\langle l_{\alpha}(t)\; l_{\beta}(t-\tau)\rangle\rangle\equiv 0, \tag{3.15}$$

then $F[\bullet]$ in equation (3.10) is *numerically* equal to equation (3.5). The problem of positivity of the KL *form* in the SL picture, using the mapping (3.14), corresponds to the positivity of the generator obtained by using the *tracing-out* technique. Within this mapping we can distinguish, once again, two particular cases:

(i) In the case of a non-hermitian U and with the selection (3.11), H_{eff} obtained from (3.12) is numerically equivalent to that of (3.4) replacing $\langle\langle l_{\alpha}^{*}(t)l_{\beta}(t-\tau)\rangle\rangle$ by $\chi_{\alpha\beta}(-\tau)$. So in this case we can write a non-Markovian SL equation which leads – in the second order approximation – to *numerically* equivalents $F[\bullet]$ and H_{eff} as those obtained from tracing-out. Note that the condition (3.15) is not necessary but it is consistent with (3.14).

(ii) In the case $U = U^\dagger$ it is not possible to make the simultaneous mapping $\langle\langle l^*_\alpha(t)\ l_\beta(t-\tau)\rangle\rangle = \chi_{\alpha\beta}(-\tau)$ and $\langle\langle l_\alpha(t)\ l_\beta(t-\tau)\rangle\rangle = \Gamma_{\alpha\beta}(-\tau)$. Then (3.15) is a consistent election leading to $H_{\text{eff}} = H_{\text{S}}$. This means that it is no possible to obtain simultaneously, for an hermitian U, both operators $F[\bullet]$ and H_{eff} as the ones coming from the tracing-out. Nevertheless the Hamiltonian term H_{eff} could always be incorporated into the dynamics of the SL, indicating that this is not a serious drawback of the SL approach with an hermitian U [3].

Other correlations that can also be useful in describing, phenomenologically, dissipative quantum systems are the Gaussian white noises

$$\langle\langle l^*_\alpha(t)\ l_\beta(t-\tau)\rangle\rangle \equiv \delta_{\alpha\beta}\delta(-\tau), \tag{3.16}$$

then leading to

$$F[\bullet] = \frac{\theta^2}{\hbar^2}\sum_\alpha V_\alpha \bullet V^\dagger_\alpha\,. \tag{3.17}$$

In this case the second order contribution gives an exact result. We note that for any operator V_α this expression guarantees the completely positive condition [1]. This is seen by writing V_α in an operator basis $\{S_\alpha\}$, which leads to a positive definite matrix $[a_{\alpha\gamma}]$ [see before equation (1.2)]. Now, from (3.16), we can split two different possibilities depending on the value of $\langle\langle l_\alpha(t)\ l_\beta(t-\tau)\rangle\rangle$.

(i) We choose $\langle\langle l_\alpha(t)\ l_\beta(t-\tau)\rangle\rangle = 0$, then $U = U^\dagger$ and $H_{\text{eff}} = H_{\text{S}}$ so the SL reads

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = \left[\frac{-\mathrm{i}}{\hbar}H_{\text{S}} - \frac{\theta}{\hbar}\sum_\alpha\left(\frac{V^\dagger_\alpha V_\alpha}{2} + \mathrm{i}l_\alpha(t)\,V_\alpha\right)\right]|\Psi\rangle \tag{3.18}$$

This equation was used by van Kampen to obtain the standard KL generator [6,11]; also Strunz [26] arrived to this stochastic equation from the Influence Functional in the Path Integral context.

(ii) We choose that (3.16) is fulfilled and in addition

$$\langle\langle l_\alpha(t)\ l_\beta(t-\tau)\rangle\rangle \equiv \delta_{\alpha\beta}\delta(-\tau), \tag{3.19}$$

then $l_\alpha(t) \in \mathcal{R}_{\text{e}}$. Now if we choose an hermitian U we get a contribution for the effective Hamiltonian of the form

$$H_{\text{eff}} = H_{\text{S}} - \mathrm{i}\frac{\theta^2}{4\hbar}\sum_\alpha\left(V^2_\alpha - (V^\dagger_\alpha)^2\right), \tag{3.20}$$

this is a consequence of allowing $\mathcal{F}(t)$ to be non-hermitian. Note that if (3.19) is fulfilled but we adopt a non-hermitian U as in (3.11) we would have gotten $H_{\text{eff}} = H_{\text{S}}$.

4. Observable q and p in the quantum master equation

In this section we describe the general form of the KL in the second order approximation for the Hamiltonian $H_{\mathrm{S}}(p,q) = p^2/2 + W(q)$, with a potential energy $W(q) = \mathcal{A}q^n$, $\mathcal{A} \geqslant 0, n = 0,1,2$. The interaction operators V_α are assumed to be a linear combination of the observables: position q and momentum p. Then the different terms in the KL *form* can be written in the general way:

$$
\begin{aligned}
F[\bullet] &= \frac{\theta^2}{\hbar^2}[2D_{pp}q \bullet q + 2D_{qq}p \bullet p + D_1 q \bullet p + D_1^* p \bullet q], && (4.1)\\
H_{\mathrm{eff}} &= H_{\mathrm{S}} - \mathrm{i}\frac{\theta^2}{2\hbar}\left(h_q q^2 + h_p p^2 + h_{pq}pq - h_{pq}^* qp\right), && (4.2)
\end{aligned}
$$

defining $\mu\hbar = \Im\mathrm{m}[h_{pq}]$ the effective Hamiltonian reads

$$
H_{\mathrm{eff}} = H_0 + \theta^2\frac{\mu}{2}(pq + qp), \tag{4.3}
$$

where $H_0 = H_{\mathrm{S}} - \mathrm{i}\theta^2(h_q q^2 + h_p p^2)/2\hbar$. Splitting the real and imaginary parts of D_1 as $2D_{qp} = \Re\mathrm{e}[D_1]$ and $-\lambda\hbar = \Im\mathrm{m}[D_1]$, the whole generator $L\,[\bullet]$ can be expressed in the form

$$
\begin{aligned}
L[\bullet] = &-\frac{\mathrm{i}}{\hbar}[H_0,\bullet] - \frac{\mathrm{i}\theta^2}{2\hbar}(\lambda+\mu)[q,\bullet p + p\bullet] + \frac{\mathrm{i}\theta^2}{2\hbar}(\lambda-\mu)[p,\bullet q + q\bullet]\\
&- \frac{\theta^2 D_{pp}}{\hbar^2}[q,[q,\bullet]] - \frac{\theta^2 D_{qq}}{\hbar^2}[p,[p,\bullet]] - \frac{\theta^2 D_{qp}}{\hbar^2}([q,[p,\bullet]] + [p,[q,\bullet]]). \quad (4.4)
\end{aligned}
$$

This generator has a KL *form* and is the most general expression, in terms of q and p, for the potential $W(q)$ and with the interaction operators V_α as mentioned before. We call D_{ij} and λ, diffusion and dissipative coefficients respectively. This kind of QME (in terms of q,p) has been analyzed by Sandulescu et al. [21] when studying the dissipation for an open harmonic oscillator. From this QME they reproduced several results that had been reported in the literature. In that reference H_0 is the Hamiltonian of the harmonic oscillator and (4.4) is obtained, phenomenologically, by proposing an interaction V being a linear combination of q and p in the KL generator (1.1).

In particular in the present work we want to analyze, from microscopic principles, these coefficients for the free particle model. Even when this system should be the simplest one we will emphasize that the quantum free particle, in interaction with a quantum reservoir, shows some controversial results in the context of a second order approximation. Hence we will try to solve certain aspects of this model.

The completely positive condition for the generator $L[\bullet]$ (4.4) is assured if the following restriction, for the coefficients, are fulfilled (see appendix C)

$$
D_{pp} > 0, \quad D_{qq} > 0, \quad D_{qq}D_{pp} - D_{qp}^2 \geqslant (\lambda^2\hbar^2/4). \tag{4.5}
$$

Note that there are two situations that (4.5) does not take into account. The first is the unitary evolution, i.e. the dissipation λ and diffusion coefficient D_{ij} vanish.

The second one corresponds to the case when only one diffusion coefficient D_{pp} or D_{qq} vanishes, while the other is positive. In this case we should have $D_{qp} = \lambda = 0$ in order to fulfil the completely positive condition. We have to mention that the fulfilment of (4.5) also assures the validity of the generalized uncertainty relation during the whole evolution of the reduced system $\mathcal{S}$ under $L[\bullet]$ [21,27,28].

In the Heisenberg representation the dual generator $L^*[\bullet]$ is defined, for any operator A, as $\mathrm{Tr}(AL[\rho]) = \mathrm{Tr}(L^*[A]\rho)$. Then the dual expression of (4.4) reads

$$\begin{aligned} L^*[\bullet] &= \frac{\mathrm{i}}{\hbar}[H_0,\bullet] - \frac{\mathrm{i}\theta^2}{2\hbar}(\lambda+\mu)([\bullet,q]p + p[\bullet,q]) + \frac{\mathrm{i}\theta^2}{2\hbar}(\lambda-\mu)(q[\bullet,p]+[\bullet,p]q) \\ &\quad - \frac{\theta^2 D_{pp}}{\hbar^2}[q,[q,\bullet]] - \frac{\theta^2 D_{qq}}{\hbar^2}[p,[p,\bullet]] - \frac{\theta^2 D_{qp}}{\hbar^2}([q,[p,\bullet]]+[p,[q,\bullet]]) \end{aligned} \tag{4.6}$$

with this generator the evolution for the moments of p, q read

$$\begin{aligned} \partial_t q^n &= \frac{\mathrm{i}}{\hbar}[H_0,q^n] - \theta^2 n(\lambda-\mu)q^n + \theta^2 n(n-1)D_{qq}q^{n-2}, \\ \partial_t p^m &= \frac{\mathrm{i}}{\hbar}[H_0,p^m] - \theta^2 m(\lambda+\mu)p^m + \theta^2 m(m-1)D_{pp}p^{m-2}, \\ \partial_t q^n p^m &= \frac{\mathrm{i}}{\hbar}[H_0,q^n p^m] - \frac{\theta^2}{2}(\lambda+\mu)m(q^n p^m + p q^n p^{m-1}) \\ &\quad - \frac{\theta^2}{2}(\lambda-\mu)n(q^n p^m + q^{n-1}p^{m-1}q) + \theta^2 n(n-1)D_{qq}q^{n-2}p^m \\ &\quad + \theta^2 m(m-1)D_{pp}q^n p^{m-2} - 2\theta^2 nmD_{qp}q^{n-1}p^{m-1}, \end{aligned}$$

in particular for the first and the second moments we obtain

$$\begin{aligned} \partial_t q &= \frac{\mathrm{i}}{\hbar}[H_0,q] - \theta^2(\lambda-\mu)q, \\ \partial_t p &= \frac{\mathrm{i}}{\hbar}[H_0,p] - \theta^2(\lambda+\mu)p, \\ \partial_t q^2 &= \frac{\mathrm{i}}{\hbar}[H_0,q^2] - 2\theta^2(\lambda-\mu)q^2 + 2\theta^2 D_{qq}\,, \\ \partial_t p^2 &= \frac{\mathrm{i}}{\hbar}[H_0,p^2] - 2\theta^2(\lambda+\mu)p^2 + 2\theta^2 D_{pp}\,, \\ \partial_t qp &= \frac{\mathrm{i}}{\hbar}[H_0,qp] - \theta^2\lambda(qp+pq) - 2\theta^2 D_{qp}\,. \end{aligned} \tag{4.7}$$

From these equations we can see a behaviour resembling the classical Brownian motion, but only in the case when $\lambda = \mu$ [28]. In the following sections we will analyze under which situation this condition can be fulfilled.

4.1. Coefficients of the KL in the second order approximation

In this section we give the structure of the coefficients appearing in (4.1) and (4.2), obtained within a second order approximation by *tracing out*, and consequently also in the SL *approach*. The interaction operators are assumed to be linear combinations of the form $V_\alpha = a_\alpha p + b_\alpha q$ with $\alpha = 1, 2$ where a_α, b_a are complex numbers (in units of $\sqrt{\hbar}$). Note that if the potential energy in H_S is $W(q) = \mathcal{A}q^n$, $(n = 0, 1, 2)$, it is easy to see that the Heisenberg evolution $V_\alpha(-\tau)$ are, once again, linear combinations, i.e.: $V_\alpha(-\tau) = \gamma_{p\alpha}(-\tau)p + \gamma_{q\alpha}(-\tau)q$, where the coefficients $\gamma_j(-\tau)$ depend on the structure of H_S. Therefore inserting this expression in (3.5) or (3.10) the dissipative coefficients of (4.1) are

$$
\begin{aligned}
D_{pp} &= \Re\mathrm{e}\left[\sum_{\alpha\beta} b_\alpha^* \int_0^\infty \mathrm{d}\tau c_{\alpha\beta}(-\tau)\gamma_{q\beta}(-\tau)\right], \\
D_{qq} &= \Re\mathrm{e}\left[\sum_{\alpha\beta} a_\alpha^* \int_0^\infty \mathrm{d}\tau\, c_{\alpha\beta}(-\tau)\gamma_{p\beta}(-\tau)\right], \\
D_1 &= \sum_{\alpha\beta}\int_0^\infty \mathrm{d}\tau \left(c_{\alpha\beta}(-\tau)\gamma_{q\beta}(-\tau)a_\alpha^* + c_{\alpha\beta}^*(-\tau)\gamma_{p\beta}^*(-\tau)b_\alpha\right), \qquad (4.8)
\end{aligned}
$$

here these coefficients are written in terms of the quantity $c_{\alpha\beta}(-\tau)$. So the correlation functions are $c_{\alpha\beta}(-\tau) = \chi_{\alpha\beta}(-\tau)$ in *tracing-out* and $c_{\alpha\beta}(-\tau) = \langle\langle l_\alpha^*(t)\; l_\beta(t-\tau)\rangle\rangle$ in the SL approach.

In the case of tracing-out (3.4), and in the SL approach when $U \neq U^\dagger$ from (3.12), the coefficients in the effective Hamiltonian can be written also in terms of $c_{\alpha\beta}(-\tau)$. Therefore we find for the coefficient of (4.2)

$$
\begin{aligned}
h_q &= 2\mathrm{i}\,\Im\mathrm{m}\left[\sum_{\alpha\beta} b_\alpha^* \int_0^\infty \mathrm{d}\tau c_{\alpha\beta}(-\tau)\gamma_{q\beta}(-\tau)\right], \\
h_p &= 2\mathrm{i}\,\Im\mathrm{m}\left[\sum_{\alpha\beta} a_\alpha^* \int_0^\infty \mathrm{d}\tau c_{\alpha\beta}(-\tau)\gamma_{p\beta}(-\tau)\right], \\
\mu\hbar &= \Im\mathrm{m}[h_{pq}] \\
&= \Im\mathrm{m}\left[\sum_{\alpha\beta}\int_0^\infty \mathrm{d}\tau \left(c_{\alpha\beta}(-\tau)a_\alpha^*\gamma_{q\beta}(-\tau) - c_{\alpha\beta}^*(-\tau)b_\alpha\gamma_{p\beta}^*(-\tau)\right)\right]. \qquad (4.9)
\end{aligned}
$$

In the case of a generator coming from SL when $U = U^\dagger$, the effective Hamiltonian (3.9) is written in terms of $\langle\langle l_\alpha(t)\; l_\beta(t-\tau)\rangle\rangle$, so the coefficients of (4.2) are

$$
\begin{aligned}
h_q &= 2\mathrm{i}\,\Im\mathrm{m}\left[\sum_{\alpha\beta} b_\alpha \int_0^\infty \mathrm{d}\tau\;\langle\langle l_\alpha(t)\; l_\beta(t-\tau)\rangle\rangle\,\gamma_{q\beta}(-\tau)\right], \\
h_p &= 2\mathrm{i}\,\Im\mathrm{m}\left[\sum_{\alpha\beta} a_\alpha \int_0^\infty \mathrm{d}\tau\;\langle\langle l_\alpha(t)\; l_\beta(t-\tau)\rangle\rangle\,\gamma_{p\beta}(-\tau)\right], \\
\mu\hbar &= \Im\mathrm{m}\left[\sum_{\alpha\beta}\int_0^\infty \mathrm{d}\tau\langle\langle l_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle a_\alpha\gamma_{q\beta}(-\tau)\right. \\
&\qquad\left. - \langle\langle l_\alpha^*(t)\, l_\beta^*(t-\tau)\rangle\rangle b_\alpha^*\gamma_{p\beta}^*(-\tau)\right]. \qquad (4.10)
\end{aligned}
$$

An explicit analysis of the results (4.8)–(4.10) will be given in the next section for a particular model.

5. The free particle

In this section we investigate the effect of the fluctuations and the dissipation for a quantum free particle in contact with an environment, which is assumed to be a set of independent harmonic oscillators with Hamiltonian H_{B} (as in section 1), then the system Hamiltonian is

$$H_{\mathrm{S}} = \frac{1}{2}p^2.$$

We are going to point out some controversial results that come from the weak coupling approximation when it is applied to this model. In the following we will consider the case where there is only one interaction operator

$$V_\alpha = V = ap + bq, \quad a, b \in \mathcal{R}_{\mathrm{e}} \tag{5.1}$$

and the interaction Hamiltonian is, once again, $H_{\mathrm{I}} = \sum_k v_k(b_k^\dagger + b_k) \otimes V$. The Heisenberg evolution of V gives $\gamma_p(-\tau) = a - b\tau$ and $\gamma_q(-\tau) = b$. The bath correlation function $\chi(-\tau)$ is given in (2.10). The Fourier transform of this correlation (see appendix B) is

$$h(\omega) = 2\pi[g(\omega)n(\omega) + g(-\omega)(n(-\omega) + 1)], \tag{5.2}$$

where $g(\omega) = \sum_k |v_k|^2 \delta(\omega_k - \omega)$ is the spectral function of a phonon bath, and we consider the Ohmic case $g(\omega) = g\ \omega$, if $0 \leqslant \omega \leqslant \Omega_{\mathrm{C}}$, where Ω_{C} is some frequency cutoff. To obtain the coefficients of (4.4) it is necessary to evaluate the integrals

$$\int_0^\infty \mathrm{d}\tau\ \chi(-\tau) = \frac{h(0)}{2} + \mathrm{i}s(0), \qquad \int_0^\infty \mathrm{d}\tau\ \chi(-\tau)\ \tau = r(0) = r^{\mathrm{R}}(0) + \mathrm{i}r^{\mathrm{I}}(0), \tag{5.3}$$

the real quantities $h(0), s(0), r^{\mathrm{R}}(0), r^{\mathrm{I}}(0)$ depend on the bath structure and its temperature β^{-1}; in appendix B there are general expressions for each of them in terms of $h(\omega)$. Using (5.3) in (4.9) we get for the Hamiltonian H_0 [see below (4.3)]

$$h_p = 2\mathrm{i}[a^2 s(0) - abr^{\mathrm{I}}(0)], \quad h_q = 2\mathrm{i}b^2 s(0) \tag{5.4}$$

and $h_{pq} = b^2 r^*(0) + \mathrm{i}2abs(0)$. The coefficients (4.8) and μ are expressed as

$$2D_{pp} = b^2 h(0), \quad 2D_{qq} = a^2 h(0) - 2abr^{\mathrm{R}}(0), \quad 2D_{qp} = abh(0) - b^2 r^{\mathrm{R}}(0),$$
$$\lambda\hbar = -b^2 r^{\mathrm{I}}(0), \quad \mu\hbar = -b^2 r^{\mathrm{I}}(0) + 2abs(0).$$

The criterium (4.5) set that the completely positive condition is satisfied only if $r(0) = 0$, and the condition to be a Brownian-like particle, $\lambda = \mu$, is fulfilled when a or b are null. From the expression $h(\omega)$ we obtain in the Ohmic case (see appendix B)

$$h(0) = 4\pi g/\beta\hbar, \quad s(0) = -g\Omega_{\mathrm{C}}\,,$$
$$r^{\mathrm{R}}(0) = -\int_0^{\Omega_{\mathrm{C}}} \mathrm{d}\omega\ [g(\omega)cth(\beta\hbar\omega/2)]'/\omega, \quad r^{\mathrm{I}}(0) = -\pi g.$$

So it can be seen that $r^{\mathrm{R}}(0)$ is well defined and it is null in the high temperature limit.

Now, let us consider the case when the free particle is located in a $1D$ box of large L; in this case there should exist an asymptotic equilibrium statistical operator $\rho^{\mathrm{eq}} = \exp(-\beta H_{\mathrm{S}})/\,\mathrm{Tr}[\exp(-\beta H_{\mathrm{S}})]$. We now can investigate which are the conditions on the coefficients in the QME in order that ρ^{eq} is the stationary state of the generator $L[\rho^{\mathrm{eq}}] = 0$. This gives the following restriction on some of the coefficients:

$$D_{pp} = (\lambda + \mu)/\beta, \quad \lambda = \mu, \quad h_q = 0. \tag{5.5}$$

The equilibrium condition does not tell anything about the other nonequilibrium coefficients. Hence it is worthwhile to see which models of the interaction will lead to the fulfilment of the condition (5.5).

Now, let us analyze the behaviour of the free particle model for two particular cases of interaction with the reservoir. The first one is when $b = 0$ in (5.1) then $V = ap$. With this particular interaction we get $2D_{qq} = a^2 h(0)$, and the effective Hamiltonian $H_0 = \frac{1}{2}p^2(1 + 2\theta^2 s(0)a^2/\hbar)$ (here $m^{-1} = (1 + 2\theta^2 s(0)a^2/\hbar)$ is a renormalized mass that is always well defined in the weak coupling approximation); the other coefficients are null $D_{pp} = D_{qp} = \lambda = \mu = 0$, so in this case the QME is completely positive because $\lambda = 0$. This generator could also be obtained, in a phenomenological way, assuming Lindblad operators of the form $V = ap$ in equation (1.1), with some temperature dependent coefficient a. This kind of interaction $V \propto p$ has also been worked in the context of path integral formalism [17]. With the help of equation (4.7) we see that the expectation of the observables, and the variance of q at long-time is not diffusive because it depends on the initial condition $p(0)$, i.e.: $q^2 = 2D_{qq}\theta^2 t + (q(0) + t\ p(0)/m)^2$. A similar behaviour was also found in the quantum random walk model [29].

A second model of interaction is when $a = 0$ in (5.1) then $V = bq$. This interaction corresponds to the most used – linear coupling – model in the path integral formalism [15,26]. Eliminating the bath variables we obtain

$$D_{qq} = 0, \quad 2D_{pp} = b^2 h(0), \quad 2D_{qp} = -b^2 r^{\mathrm{R}}(0), \quad h_q = 2\mathrm{i}b^2 s(0), \tag{5.6}$$
$$\mu\hbar = \lambda\hbar = -b^2 r^{\mathrm{I}}(0) > 0$$

and $H_0 = p^2/2 - \theta^2 g\Omega_{\mathrm{C}} b^2 q^2/\hbar$. At high temperatures $2D_{qp} = -b^2 r^{\mathrm{R}}(0) \to 0$ so the QME (2.12) is reobtained (with $\gamma = g\pi/\hbar$). A similar QME was also given in [30] where they called the approach *the* “Non-rotating wave approximation” (NRW). In that work the QME is obtained eliminating the bath variables in the Heisenberg representation, but neglecting the additional spurious term $\theta^2 g\Omega_{\mathrm{C}} b^2 q^2/\hbar$ in H_0. Now we can analyze the characteristics of the present model. The first remarkable fact is that the diffusion coefficient D_{qq} vanishes but the dissipative coefficient λ does not, giving therefore – from (4.5) – a generator which is not a bonafide KL; even more at high temperatures – in the second order approximation – the generator (2.12) is not completely positive. Note that the problem of non-positivity in a second order approximation and with an interaction $V \sim q$ can not be solved considering intermediate temperatures; in order to overcome this problem other approximations must be made [19]. What is even more problematic in the (Ohmic) second order approximation and at high temperatures, is the additional quadratic spurious term $\theta^2 s(0) b^2 q^2/\hbar$. This gives rise to a non-physical contribution for the effective free particle Hamiltonian (if H_{S} represented an harmonic oscillator the spurious term could be considered a shift, i.e. a renormalization frequency). This is a serious drawback of the Born-Markov approximation, for the free particle model, because this term can not be neglected in this context. On the other hand from (5.6) $\mu = \lambda$, so the system behaves like a Brownian quantum particle. From the point of view of an equilibrium state, see (5.5), if we had $h_q = 0$ the equilibrium state ρ^{eq} would be the stationary point of the generator. Note also that if we could neglect the spurious term in H_0 and in the limit of high temperatures ($D_{qp} \to 0$), from equations (4.7) and (5.6) a diffusive behaviour $q^2 \sim D_{pp} t/4\lambda$ would be obtained at long times. In the following sections we overcome – phenomenologically – the problems of non-positivity and spurious term in the Hamiltonian H_0, always preserving the character of a quantum Brownian-like motion.

5.1. Using the Shrödinger-Langevin approach

Now we want to analyze which stochastic state vector could reproduce the behaviour of a free particle in contact with a thermal bath, with interaction $V = bq$. Therefore this section is twofold: the first one is concerned with Caldeira and Leggett's QME at infinite temperature (2.12); in the second part we present a SL equation which reproduces a completely positive QME for the Brownian free particle at finite temperature; therefore we will use some of the coefficients of (5.6) but the others will be changed in order to obtain a positive KL *form*. In addition we handle the problem of the extra spurious term in H_0 and preserve the Brownian-like dynamics. In order to go on with this program we are going to choose suitable correlation functions in the SL picture. Our point of view has a similar purpose as in the paper [20] where a phenomenological approach to Caldeira and Leggett's QME was presented. In that work Gao used a particular Lindblad operator V (at a finite temperature) in (1.1) in order to obtain a stochastic differential equation [10] that reaches Caldeira and Leggett's QME at infinite temperatures. Unfortunately Gao's approach gives a non-hermitian effective Hamiltonian and the dynamics of p and q does not correspond to a Brownian-like motion [31].

5.1.1. The Caldeira and Leggett QME ($\beta \to 0$)

Let us introduce the *exact* stochastic state equation that represents the evolution of the Caldeira and Leggett's QME. To do this we go back to section 3.2 and assume a stochastic operator $\mathcal{F}(t) = l(t)V$ with interaction $V = q$ and $l(t)$ a complex-value Gaussian noise. Using the correlation mapping (3.14) with $\chi_\infty(-\tau)$ (i.e.: $< l^* l(-\tau) >= (2\gamma/\beta)\delta(\tau) + \mathrm{i}\gamma\hbar\delta'(\tau)$ and $< ll(-\tau) >= 0$), and taking a *non-*

hermitian U, from (3.11) we obtain that the SL equation has the form

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = \left[\frac{-\mathrm{i}}{\hbar}H_{\mathrm{S}} - \frac{\theta}{\hbar}\left(\theta\gamma\left[q^2\left(-\mathrm{i}\tilde{\delta}(0)+\frac{1}{\hbar\beta}\right)-\mathrm{i}\frac{qp}{2}\right]+\mathrm{i}l\,(t)\,q\right)\right]|\Psi\rangle\,. \tag{5.7}$$

This exact equation represents a quantum system under the evolution of (2.12) and gives a diffusion behaviour at long times. In this form (5.7) gives the same $F[\bullet]$ [once again not fulfilling (4.5)] and H_{eff} as in (2.12).

We note that if U were *hermitian* the SL dynamics, considering the same $\mathcal{F}\,(t)$ and correlation mapping as before, would have given $F[\bullet]$ with coefficients D_{pp}, D_{qq}, D_{qp}, λ as in (5.6) for $\beta\to 0$, but in this case $H_{\mathrm{eff}} = H_{\mathrm{S}}$ so $\mu = 0$. Therefore the observables p, q would have shown damping in the velocity and in the position, i.e.: $\dot{q} = p - \lambda q$ and $\dot{p} = -\lambda p$. At long times the behaviour of the second moment of the position is subdiffusive $q^2 \sim D_{qq}/2\theta^4\lambda^3$ and $p^2 \sim D_{qq}/\lambda$, so giving finite dispersion at infinite times. Hence if $U = U^{\dagger}$ the SL dynamics of the system is not completely equivalent to that of *tracing-out.* As expected we see that the inclusion of the effective Hamiltonian (4.3) gives a non-trivial contribution to the dissipative dynamics. We note that, as was mentioned in section 3.2, using an hermitian U and stochastic $c-$numbers $l_\alpha(t)$ it is not possible to map the superoperator $F[\bullet]$ and consistently the effective Hamiltonian from tracing-out. This fact can only be solved using the phenomenological Hamiltonian

$$H_{\mathrm{eff}} = p^2/2 + \theta^2\mu(pq+qp)/2 \tag{5.8}$$

with $\mu = \lambda$.

5.1.2. The QME at a finite temperature

Now let us work out two models in the context of the SL picture with $U = U^{\dagger}$, from which it is possible to reproduce the behaviour of a quantum Brownian free particle at a finite temperature. In addition we fulfil the completely positive condition on the QME and eliminate the spurious term.

Model (1): Here we take the stochastic operator $\mathcal{F}\,(t) = apl_1(t) + bql_2(t)$ (a, b are real parameters) with colour noises $l_\alpha(t)$. So we have two correlation functions to be defined $\langle\langle l_\alpha^*\,(t)\; l_\beta\,(t-\tau)\rangle\rangle = \delta_{\alpha\beta}\; c_{\alpha\alpha}(-\tau)$ for $\alpha = 1, 2$ with $\langle\langle l_\alpha\,(t)\; l_\beta\,(t-\tau)\rangle\rangle = 0$. If $h_\alpha(\omega)$ is the Fourier transform of $c_{\alpha\alpha}(-\tau)$, see appendix B, the coefficients of $F[\bullet]$ are:

$$2D_{qq} = a^2h_1(0),\;\; 2D_{pp} = b^2h_2(0),\;\; 2D_{qp} = -b^2r_2^{\mathrm{R}}(0),\;\; \lambda\hbar = -b^2r_2^{\mathrm{I}}(0)\;, \tag{5.9}$$

comparing with (5.6) we can choose $h_2(\omega) = h(\omega)$ from (5.2), and $h_1(\omega)$ in such a way to assure the completely positive condition and also to get that $h_1(0)$ goes to zero for $\beta\to 0$. Hence using (4.5) the following inequality must be satisfied

$$a^2h_1(0)h_2(0) \geqslant b^2(r_2(0))^2. \tag{5.10}$$

In order to have a Brownian-like dynamics we have to introduce the phenomenological effective Hamiltonian (5.8). With the correlations previously introduced we now have a colour linear stochastic dynamics that reproduces the non-Markovian behaviour for a free particle in a reservoir.

Model (2): In this case we propose $\mathcal{F}(t) = \sum_\alpha l_\alpha(t)V_\alpha$, with $V_\alpha = a_\alpha p + b_\alpha q$, $\alpha = 1, 2, \cdots$ and assume white noise correlations as defined in (3.16) and (3.19). Then we obtain from (3.17) and (3.20) the coefficients

$$\begin{aligned} 2D_{pp} = \textstyle\sum_\alpha |b_\alpha|^2, \quad 2D_{qq} = \sum_\alpha |a_\alpha|^2, \quad 2D_{qp} = \sum_\alpha \Re\mathrm{e}(b_\alpha a_\alpha^*), \\ h_q = \mathrm{i}\textstyle\sum_\alpha \Im\mathrm{m}({b_\alpha}^2), \quad h_p = \mathrm{i}\sum_\alpha \Im\mathrm{m}({a_\alpha}^2), \\ \lambda\hbar = -\textstyle\sum_\alpha \Im\mathrm{m}(b_\alpha a_\alpha^*), \quad \mu\hbar = \sum_\alpha \Im\mathrm{m}(b_\alpha a_\alpha). \end{aligned} \tag{5.11}$$

Now we can play around with these coefficients in order to fulfil all the requirements mentioned before. In order to have a proper free particle Hamiltonian $H_0 = p^2/2$, i.e.: with $h_q = 0$, we can choose $b_\alpha \in \mathcal{R}_\mathrm{e}$; now to get $\mu = \lambda$ we choose $\Im\mathrm{m}(a_\alpha) \neq 0$. In this case the completely positive condition is fulfilled for any b_α, a_α (as we saw in section 3.2). The simplest case corresponds to $\alpha = 1$, then comparing (5.11) with the coefficients from (5.6), and using (4.5) we obtain for the parameters:

$$b = \sqrt{\frac{4\pi g}{\beta\hbar}}, \qquad a = \sqrt{\frac{\beta\hbar}{4\pi g}}(-r^\mathrm{R}(0) + \mathrm{i}\pi g).$$

We remark that in this case we get a completely positive KL *form*, which in addition in the high temperature limit $\beta \to 0$ represents – in the second order approximation– the situation of (2.12). Then our SL equation, with white noise correlations, also provides a good tool to reproduce the behaviour of a free particle in a reservoir at a finite temperature.

6. Discussion

In this work we review the Markovian approximation for the evolution of an open quantum system in contact with a thermal bath. We analyze the quantum master equation by using Terwiel's cumulants and the projector operator technique. Taking into account an infinite set of harmonic oscillators (the bath), we have compared our solution with the propagator of the reduced density matrix obtained from the path integral approach. We have revisited in a second order approximation the Kossakowski-Lindblad *form* for the generator. We have also presented – in a phenomenological approach – the quantum master equation obtained from the Schrödinger-Langevin picture; this was written in terms of a dissipative operator U and some stochastic operator $\mathcal{F}(t)$. For the case when U is non-hermitian we have been able to present a non-Markovian wave function whose Kossakowski-Lindblad *form* completely matches the H_eff and $F[\bullet]$ as obtained from tracing-out in a second order approximation. This procedure is a helpful tool since the state vector is simpler to handle than the density matrix. The second order weak coupling approximation – for these two formalisms – is applied to systems with potentials $W(q) = \mathcal{A}q^n, n = 0, 1, 2$ and when the interacting operators V_α are linear combination of the momentum p and position q.

The Kossakowski-Lindblad *form* for a free particle interacting with a thermal environment has been analyzed. Eliminating the bath variables a Brownian-like behaviour is obtained although the generator does not satisfy the "structural theorem", when $V = q$. Therefore in the context of the Schrödinger-Langevin picture, we present a phenomenological treatment in order to produce the Brownian dynamics and to obtain a bonafide KL. The stochastic wave function for the free particle has been introduced in section 5.1. In section 5.1.1 we show the Schrödinger-Langevin picture that exactly represents the dynamics given by the Caldeira and Leggett quantum master equation. We also noted the role of the effective Hamiltonian, which leads to an important contribution to the dissipative behaviour. In section 5.1.2 we consider two models of dynamics. In model (1) we show a non-Markovian state vector, for the free particle, which matches (in a second order approximation) the behaviour given by the Kossakowski-Lindblad generator. In this case the correct free particle Hamiltonian is obtained by adding the phenomenological term (5.8). In model (2) the dynamics is controlled by white noises, then by selecting suitable parameters a Brownian-like behaviour is obtained. In this case the spurious term is automatically eliminated and the generator is always a bonafide KL. In both models the thermal wave function is given at a finite temperature, so this approach is useful to analyze the individual realizations of the dissipative system.

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A. Terwiel and ordered cumulants

In this section we briefly review the theory of the Terwiel cumulants [22] in order to obtain the Markovian equation (2.8). Using the definitions of the section 1, we start in the interaction representation:

$$\dot{\sigma}_{\mathrm{T}} = \theta \mathcal{L}_{\mathrm{I}}(t)\sigma_{\mathrm{T}},$$

and define the projector operator that eliminates the bath variables [6,25]

$$\mathcal{P}[\bullet] \equiv \rho_{\mathrm{B}}\,\mathrm{Tr}_{\mathrm{B}}[\bullet],$$

the reduced density matrix is obtained as $\mathcal{P}\sigma_{\mathrm{T}} = \rho_{\mathrm{B}} \otimes \sigma_{\mathrm{S}}$, projecting at *any time* the total density matrix into the tensorial product of the equilibrium distribution of the bath times the reduced density matrix of $\mathcal{S}$. Then it is possible to write the evolution equations for $\mathcal{P}\sigma_{\mathrm{T}}$ and $(1-\mathcal{P})\sigma_{\mathrm{T}}$ as

$$\frac{\mathrm{d}(\mathcal{P}\sigma_{\mathrm{T}})}{\mathrm{d}t} = \theta\mathcal{P}\mathcal{L}_{\mathrm{I}}(t)(1-\mathcal{P})\sigma_{\mathrm{T}}, \tag{A.1}$$

$$\frac{\mathrm{d}((1-\mathcal{P})\sigma_{\mathrm{T}})}{\mathrm{d}t} = \theta\mathcal{L}_{\mathrm{I}}(t)\mathcal{P}\sigma_{\mathrm{T}} + \theta(1-\mathcal{P})\mathcal{L}_{\mathrm{I}}(t)(1-\mathcal{P})\sigma_{\mathrm{T}}. \tag{A.2}$$

Equation (A.2) can formally be solved and its solution be substituted in (A.1) yielding an exact integro differential equation for σ_{S}

$$\dot{\sigma}_{\mathrm{S}} = \theta^2 \int_0^t k(t|t')\ \sigma_{\mathrm{S}}(t')\mathrm{d}t' = \theta^2 \int_0^t \langle \mathcal{L}_{\mathrm{I}}(t) T(t|t') \mathcal{L}_{\mathrm{I}}(t') \rangle_{\mathrm{B}}\ \sigma_{\mathrm{S}}(t')\mathrm{d}t', \qquad \text{(A.3)}$$

where $T(t|t')$ itself satisfies the Green equation

$$\dot{T}(t|t') = \theta(1-\mathcal{P})\mathcal{L}_{\mathrm{I}}(t)T(t|t') \qquad (t \geqslant t')$$

with initial condition $T(t|t) = 1$. Hence (A.3) is the starting point to perform a Markovian approximation. First it is possible to express $k(t|t') = \sum_{n=2}^{\infty} k_n(t|t')$ where $k_2(t_1|t_2) = \langle \mathcal{L}_{\mathrm{I}}(t_1)\mathcal{L}_{\mathrm{I}}(t_2)\rangle_{\mathrm{B}}$ and the general n^{th} order term is given by

$$k_n(t_1|t_n) = \theta^{n-2} \int_{t_n}^{t_1} \mathrm{d}t_2 \int_{t_n}^{t_{n-2}} \mathrm{d}t_{n-1} \langle \mathcal{L}_{\mathrm{I}}(t_1)(1-\mathcal{P})\mathcal{L}_{\mathrm{I}}(t_2)\cdot\cdot\mathcal{L}_{\mathrm{I}}(t_{n-1})(1-\mathcal{P})\mathcal{L}_{\mathrm{I}}(t_n)\rangle_{\mathrm{B}}$$

for $n = 3, 4, 5...$ The term in brackets, inside the integrals, is known as Terwiel's cumulant and it can be shown that it vanishes when two successive times fulfil $|t_i - t_{i+1}| > \tau_{\mathrm{c}}$ where τ_{c} is the correlation time of the bath, so the n^{th} order contribution to $k(t|t')$, in (A.3), is of the order $\theta(\theta\tau_{\mathrm{c}})^{n-1}$ therefore leading to a well ordered expansion. Equation (A.3) is exact and it still has a non-Markovian behaviour. In order to find a closed Markovian equation, like in (2.8), it is necessary to take into account the "memory terms". Then the final expression is

$$\dot{\sigma}_{\mathrm{S}} = \sum_{n=2}^{\infty} \theta^n K_n\, \sigma_{\mathrm{S}}(t).$$

Note that we have used $\langle \mathcal{L}_{\mathrm{I}}(t)\rangle_{\mathrm{B}} = 0$ which is the case in most applications and $K_n(t)$ is given by (2.7) which is written in terms of the *ordered* cumulants

$\langle \mathcal{L}_{\mathrm{I}}(t)\mathcal{L}_{\mathrm{I}}(t_1)\cdots\mathcal{L}_{\mathrm{I}}(t_{n-1})\rangle_{\mathrm{B}}^p$ as defined by Terwiel [22], Fox[23] and van Kampen [6]. Then the K_n contribution is also of the order $\theta(\theta\tau_{\mathrm{c}})^{n-1}$ and when $t \gg \tau_{\mathrm{c}}$ it can be written in the form $K_n = K_n(\infty)$. In this way we obtain the Markovian approximation for the evolution of the reduced system, but not precisely a bonafide KL.

B. Handling the correlation functions

Here we show how to calculate the coefficients (5.3) in terms of the Fourier transform of the correlation function. Let us use the fact that

$$\int_0^{\infty} \exp(\mathrm{i}\omega\tau)\,\mathrm{d}\tau = \pi D(\omega) + \mathrm{i}P(\omega), \qquad \int_0^{\infty} \tau\ \exp(\mathrm{i}\omega\tau)\,\mathrm{d}\tau = -\mathrm{i}\pi D'(\omega) + P'(\omega), \quad \text{(B.1)}$$

where $D(\omega)$ and $P(\omega)$ are distributions acting in the following way

$$\int_{-\infty}^{\infty} f(\omega)\ D(\omega)\ \mathrm{d}\omega = f(0), \qquad \int_{-\infty}^{\infty} f(\omega)\ D'(\omega)\ \mathrm{d}\omega = -f'(0),$$

$$\int_{-\infty}^{\infty} f(\omega)\ P(\omega)\ \mathrm{d}\omega = \mathcal{VP}\int_{\infty}^{\infty} \frac{f(\omega)}{\omega}\ \mathrm{d}\omega, \qquad \int_{-\infty}^{\infty} f(\omega)\ P'(\omega)\ \mathrm{d}\omega = -\mathcal{VP}\int_{\infty}^{\infty} \frac{f'(\omega)}{\omega}\ \mathrm{d}\omega,$$

$\mathcal{VP}$ in front of the integrals mean Cauchy principal values. The Fourier transform of $c(-\tau)$ is

$$h(\omega) = \int_{-\infty}^{\infty} c(-\tau)\ \exp(-\mathrm{i}\omega\tau)\ \mathrm{d}\tau, \qquad c(-\tau) = \frac{1}{2\pi}\int_{-\infty}^{\infty} h(\omega)\ \exp(\mathrm{i}\omega\tau)\ \mathrm{d}\omega, \tag{B.2}$$

$h(\omega) \in \mathcal{R}_{\mathrm{e}}$ is a real function because of the stationary property of the quantum correlation functions $c(-\tau) = c^*(\tau)$. Now the following half-Fourier transforms are frequently used in the definitions of QME's coefficients

$$\int_{0}^{\infty} c(-\tau)\ \exp(-\mathrm{i}\omega\tau)\ \mathrm{d}\tau \ = \ \frac{h(\omega)}{2} + \mathrm{i}s(\omega), \tag{B.3}$$

$$\int_{0}^{\infty} \tau c(-\tau)\ \exp(-\mathrm{i}\omega\tau)\ \mathrm{d}\tau \ = \ r(\omega) = r^{\mathrm{R}}(\omega) + \mathrm{i}r^{\mathrm{I}}(\omega) \tag{B.4}$$

with $s(\omega), r^{\mathrm{R}}(\omega), r^{\mathrm{I}}(\omega) \in \mathcal{R}_{\mathrm{e}}$. We can find expressions for these real and imaginary parts of the half-Fourier transform in terms of $h(\omega)$; inserting (B.2) in (B.3) and using relations (B.1) we can write the Kramers-Kronig like relation

$$s(\omega) = \frac{1}{2\pi}\mathcal{VP}\int_{-\infty}^{\infty} \frac{h(\omega')}{\omega' - \omega}\ \mathrm{d}\omega' = \frac{1}{2}\mathcal{H}[h(\omega')]_{\omega'=\omega}\ ,$$

where $\mathcal{H}[\bullet]$ is the Hilbert transform. The real and imaginary part of $r(\omega)$ are found inserting (B.2) in (B.4) and again using some of the relations (B.1)

$$r^{\mathrm{R}}(\omega) = -\frac{1}{2\pi}\mathcal{VP}\int_{-\infty}^{\infty} \frac{h'(\omega')}{\omega' - \omega}\ \mathrm{d}\omega' = -\frac{1}{2}\mathcal{H}[h'(\omega')]_{\omega'=\omega}, \qquad r^{\mathrm{I}}(\omega) = \frac{h'(\omega)}{2}.$$

If $c(-\tau)$ are real functions the stationary condition implies $c(-\tau) = c(\tau)$, leading not only to a real but also to an even Fourier transform $h(\omega) = h(-\omega) \in \mathcal{R}_{\mathrm{e}}$. Because of this, the imaginary parts of the half-Fourier transform takes, at zero frequency, the value $s(0) = r^{\mathrm{I}}(0) = 0$ [13].

C. The completely positive condition

In this appendix we show how the inequalities (4.5) can be derived. These conditions on the coefficients of the KL *form* assure the validity of the structural theorem.

Following the lines of [21], let us propose phenomenological operators $V_i = a_i p + b_i q$ – with $i = 1, 2$ and a, b complex numbers – in the KL generator (1.1). Therefore the dissipative superoperator takes the form

$$F[\bullet] = \sum_{i=1}^{2} V_i \bullet V_i^\dagger = \sum_{i=1}^{2} \left[|a_i|^2 p \bullet p + |b_i|^2 q \bullet q + a_i^* b_i \; q \bullet p + b_i^* a_i \; p \bullet q \right] . \qquad \text{(C.1)}$$

The coefficients fulfil

$$\sum_{i=1}^{2} |a_i|^2 > 0, \qquad \sum_{i=1}^{2} |b_i|^2 > 0$$

and using the Shwartz inequality we get

$$\left| \sum_{i=1}^{2} a_i^* b_i \right|^2 = \left(\Re\mathrm{e} \left[\sum_{i=1}^{2} a_i^* b_i \right] \right)^2 + \left(\Im\mathrm{m} \left[\sum_{i=1}^{2} a_i^* b_i \right] \right)^2 \leqslant \sum_{i=1}^{2} |a_i|^2 \sum_{i=1}^{2} |b_i|^2 .$$

Identifying $\sum_{i=1}^{2} |a_i|^2 = 2D_{qq}$, $\sum_{i=1}^{2} |b_i|^2 = 2D_{pp}$, $\sum_{i=1}^{2} a_i^* b_i = 2D_{qp} - \mathrm{i}\lambda\hbar$ the above inequalities lead to the restrictions (4.5) as stated by [21]. This condition can also be obtained if we consider the operator basis $\{q, p\}$ and write the matrix $[a_{ij}]$ – defined in the introduction – corresponding to (C.1) in that basis. Then condition (4.5) appears if we ask to the matrix $[a_{ij}]$ to be positively definite.

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Квантова дисипація та феноменологічні підходи

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Перевіряється придатність використання Тервіелових кумулянтів у Марковському наближенні для отримання квантового "фундаментального кінетичного рівняння" для системи, що взаємодіє з термічним середовищем. Проаналізовано друге наближення за слабкою константою взаємодії та подається форма Косаковського–Ліндблада для ґенераторів у термінах операторів координат та імпульсів. Опрацьовано друге наближення за слабкою константою взаємодії для стохастичної немарковської хвильової функції. Досліджується модель вільних частинок, що взаємодіють із квантовим термічним середовищем, у рамках картини Шредінґера–Ланжевена. Для того, щоб обійти певні труднощі в часовій еволюції для вільночастинкового гамільтоніана у другому наближенні, вводиться феноменологічна точка зору.

Ключові слова: *відкриті квантові системи, квантове фундаментальне кінетичне рівняння, стохастичне рівняння Шредінґера*

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