The quantum master equation revisited

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For quantum open systems the semigroup approach in the weak coupling approximation has been revisited. We have proved that tracing-out the bath variables a generator of the Kossakowski-Lindblad *form* is always obtained. This fact does not guarantee the completely positivite condition. Nevertheless, in terms of the interaction Hamiltonian we have stressed the relevance of the invariance under Davies's average procedure in order to arrive to a *completely positive* semigroup. The alternative approach called the Schrödinger-Langevin picture has been introduced. Then a non-Markovian evolution equation for a *stochastic state vector* has been presented. In the context of a perturbation theory in the Kubo number, the average over the noises leads to a dissipative generator which has formally a Kossakowski-Lindblad *form*. In this context it is possible to find noise correlation functions to guarantee the completely positive condition. The equivalence of this picture with the *trace-out* technique in the weak coupling approximation has been proved. The benefit of the Schrödinger-Langevin picture to work-out with a *stochastic state vector* representing a thermal ensemble has been pointed out.

Keywords: Quantum open systems; stochastic Schrödinger equation; non-Markovian

En la aproximación de acoplamiento débil, el esquema de semigrupo para un sistema cuántico abierto ha sido reanalizado. Nosotros probamos que eliminando las variables del baño siempre se obtiene un generador de la *forma* de Kossakowski-Lindblad. Este hecho no garantiza la condición de completamente positivo. Sin embargo, en términos del hamiltoniano de interacción nosotros hemos enfatizado la relevancia de la invarianza bajo el procedimiento del promedio de Davies para así arribar a un semigrupo completamente positivo. El esquema alternativo llamado representación de Schrödinger-Langevin ha sido introducido. De esta manera, una ecuación de evolución no-markoviana para el vector de estado estocástico ha sido presentada. En el contexto de una teoría de perturbación en el número de Kubo, el promedio sobre los ruidos lleva a un generador de disipación, el cual tiene formalmente la *forma* de Kossakowski-Lindblad. En este contexto es posible encontrar funciones de correlación del ruido que garanticen la condición de completamente positivo. La equivalencia de esta representación con la técnica de eliminación de variable en la aproximación de acoplamiento débil ha sido probada. El beneficio de trabajar en la representación de Schrödinger-Langevin con un vector de estado estocástico para representar un ensamble térmico ha sido remarcado.

Descriptores: sistemas cuánticos abiertos; equación estocástica de Schrödinger; no Markoviano

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1. Introduction

In classical physics it is well accepted, within the Markovian stochastic description [1], that the master equation is an excellent approximation to describe fluctuation and dissipation at the mesoscopic level. In quantum mechanics the most general form of a Markovian evolution for the reduced density matrix $\rho(t)$, that give rise to irreversibility, is less popular. Unfortunately sometimes the epithet "Markov" is used with regrettable looseness. A Markov evolution (*i.e.*, a quantum semigroup) has to guarantee that $\rho(t)$ be hermitian positive definite with unit trace at all time, *i.e.*, von Neumann's conditions.

The Markovian map has been well established long time ago $[2,3]$ and its generator is the so called Kossakoswki-Lindblad (K-L) one. This generator gives a Markovian map that guarantees von Neumann's conditions on $\rho(t)$, and also provides a completely positive map on trace class operators $\mathcal{T}$. This last condition is much stronger than the usual positivity[a]

The Lindblad dissipative generator [3] is frequently written on a Banach space in its diagonal *standard* representation; the Kossakowski one [2] is more familiar (in physics literature) because it is written for finite dimensional systems [4].

In an arbitrary finite dimensional Hilbert space $\mathbf{H}_S$ ($\dim \mathbf{H}_S = N$) the dissipative K-L generator (*i.e.* subtracting any possible von Neumann term) is

$$L_D[\bullet] \equiv \frac{1}{2}\sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma}\left([V_\alpha\bullet, V_\gamma^\dagger] + [V_\alpha, \bullet V_\gamma^\dagger]\right),$$

(acts on $\mathcal{T}$), where V_α, $\alpha = 0, 1, \cdots, N^2-1$ is a basis in the C^* algebra of the $N \times N$ complex matrix $\mathcal{M}(N)$, $V_0 = \mathbf{1}$, and $a_{\alpha\gamma}$ is a hermitian positive-definite matrix characterizing the dissipation and the fluctuations of an *open* quantum system (from now on we will call $a_{\alpha\gamma}$ the *algebraic structure*). Earlier comments on the positiveness of the solution of the quantum master equation, in the context of nonequilibrium spontaneous emission, can be seen in Agarwal's book and references therein [5].

How to construct the K-L generator for a given open quantum system is another task. In principle we wish to find the K-L generator from the underlying hamiltonian dynamics for the *total closed system* (our system of interest $\mathcal{S}$ plus a bath $\mathcal{B}$) but sooner or later this is often technically impossible and therefore one needs to introduce *some approximations* in order to arrive to the quantum master equation.

In general, by tracing out the bath variables it does not lead to a quantum semigroup [6, 7]. It is noticeable to remark that if we deal with this situation it is always possible to introduce a *mathematical device*—due to Davis [6]—which leads to a K-L generator. From Davies's averaging procedure, in the weak coupling approximation (applied to the differential equations of motion), and when the hamiltonian of the reduced system is nondegenerate, the evolution of the diagonal elements of the reduced density matrix ρ are uncoupled from off-diagonal ones, so the dynamics of the evolution is reduced to a classical Pauli master equation for $\rho_{jj} \equiv < j \mid \rho \mid j >$.

The purpose of the present work is twofold. In the first part of the paper we are concerned with the characterization of the K-L generator (its effective hamiltonian $H_{\rm eff}$ and dissipative part $L_D[\bullet]$). Foremost, we will show that *tracing out* the bath variables—in the weak coupling approximation—*always* leads to a K-L *form*. Nevertheless we will remark that a K-L *form* does not mean that the *algebraic structure* $a_{\alpha\gamma}$ will be positive-definite. To assure this fact there will be a second step in the procedure, which strongly depends on the interaction hamiltonian H_I between $\mathcal{S}$ and $\mathcal{B}$. With this purpose we will explore the invariance under Davies's averaging procedure. In this form we will be able to give, in the weak coupling approximation, a sufficient condition—in the interaction hamiltonian—in such a way to produce a bonafidė K-L *form* from the underlying dynamics of the *total closed system*. Some examples are given in the context of spin-boson systems.

Different ways of writing the K-L generator are shown in appendix A. This fact also enlightens some difficulties posed by van Kampen and Oppenheim [8] in arriving to a K-L *form* from tracing-out the bath variables.

The second part of our paper is about the Schrödinger-Langevin picture and its connection with K-L generators. In Sect. 5 we will present an analysis concerning their similarities and differences with others alternative stochastic formulations for quantum dissipative theories [1, 9–15]. The present picture gives the evolution equation for a *stochastic state vector*, which represents a quantum open system. Then any statistical average obtained from $\rho(t)$ can alternatively be taken by introducing an average over the thermal ensemble of wave functions. A clear interpretation of the non-Markovian evolution equation for the *stochastic state vector*, in terms of random operators, will also be given.

From this stochastic state vector we obtain the evolution equation for the stochastic matrix $\rho_{st}(t)$, from which its mean value corresponds to the reduced density matrix of $\mathcal{S}$. Taking this average—over the noises—in the context of a perturbation theory in the Kubo number, a dissipative generator of the K-L *form* appears. Then we will be able to interpret, in the weak coupling approximation, the responsible of the dissipation and the fluctuating terms appearing in a K-L *form*. Therefore from the Schrödinger-Langevin picture it will be possible to build up several K-L generators from a family of correlation functions. In this way (as soon as the basis on the Hilbert space $\mathbf{H}_S$ is chosen) the correlations of the noises can be selected, in an empirical way, to represent different physical situations and at the same time to assure a positive structure $a_{\alpha\gamma}$. A simple example is when the noises are white, then it is easy to see that the hamiltonian shift cancels out and the dissipative generator will be the corresponding *standard* K-L semigroup [1, 9, 10, 12].

Also the rigorous equivalence of our stochastic picture with the *trace-out* techniques will be proved [17]. We emphasize that, in this case, the positivity or not of the algebraic structure of the K-L *form* is something that depends on the type of interaction with the bath, so its analysis belongs to the section concerning the invariance under Davies's device (Sect. 4). In terms of the Schrödinger-Langevin picture this means that if we want to match with the trace-out technique, the positivity of $a_{\alpha\gamma}$ depends on the class of interaction hamiltonian H_I from which the noise correlation function can be read off.

Another advantage from the Schrödinger-Langevin picture comes from a reverse point of view. Assume that we know a given algebraic structure $a_{\alpha\gamma}$ to be positive, then we can wonder which could be the set of noises in such a way to produce the same dynamics. This task can be solve in the present formalism, see Sect. 5.5.

In the same spirit as with the non-linear stochastic equation for the state vector [12], and in the quantum-jump model [18], our wave-function thermal approach to dissipative processes gives a suitable tool to tackle numerically complex systems.

2. The quantum dissipative semigroup

The quantum dynamical semigroup in the Schrödinger picture reads from ($\hbar = 1$)

$$\frac{d\rho(t)}{dt} = K[\rho(t)]$$

$$\equiv -i[H_{\rm eff}, \rho(t)] + \frac{1}{2}\sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma}([V_\alpha, \rho(t)V_\gamma^\dagger] + [V_\alpha\rho(t), V_\gamma^\dagger]), \tag{1}$$

while for the Heisenberg dynamics the dual generator[b] $K^*[\bullet]$

is given from

$$\frac{dA(t)}{dt} = K^*[A(t)]$$
$$\equiv i[H_{\text{eff}}, A(t)] + \frac{1}{2}\sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma}(V_\gamma^\dagger[A(t), V_\alpha] + [V_\gamma^\dagger, A(t)]V_\alpha), \quad (2)$$

where H_{eff} is some effective hamiltonian acting on the reduced system $\mathcal{S}$. As we mentioned before a necessary and sufficient condition to guarantee the completely positive condition is $a_{\alpha\gamma} \geq 0$. Summarizing, the semigroup (1) [or (2)] is the only candidate for a dynamical map describing a Markovian irreversible evolution of open quantum systems in the Schrödinger [or Heisenberg] picture [4].

Remark 1. These generators can trivially be written in the form

$$\frac{d\rho(t)}{dt} = -i[H_{\text{eff}}, \rho(t)] - \{D, \rho(t)\}_+ + F[\rho(t)], \quad (3)$$

where $\{\cdot,\cdot\}_+$ denotes the anticommutator. The dual dynamics would be

$$\frac{dA(t)}{dt} = i[H_{\text{eff}}, A(t)] - \{D^*, A(t)\}_+ + F^*[A(t)], \quad (4)$$

where

$$D = \frac{1}{2}\sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma} V_\gamma^\dagger V_\alpha, \qquad D^* = D \quad (5)$$

will be called the *dissipative* operator and

$$F[\bullet] = \sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma} V_\alpha \bullet V_\gamma^\dagger,$$
$$F^*[\bullet] = \sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma} V_\gamma^\dagger \bullet V_\alpha \quad (6)$$

the *fluctuating* superoperators. Here, as before, $F^*[\bullet]$ represents the dual. An interpretation of D and the fluctuating superoperator $F[\bullet]$ will be shown in Sects. 4 and 5. This splitting is frequently used in the context of the Quantum Jump approach [15].

Let us now see (3) from a formal point of view. Its solution could be written in the form

$$\rho(t) = \exp\left(-t\{D,\bullet\}_+\right)\rho(t_o) + \int_0^{t-t_o} \exp\left(-\tau\{D,\bullet\}_+\right) \times \left(-i[H_{\text{eff}},\bullet] + F[\bullet]\right)\rho(t-\tau)\, d\tau \quad (7)$$

Then the dynamics will erase the initial condition $\rho(t_o)$ only if D is a positive operator; this of course is guarantee by (5).

3. Tracing over the bath (weak coupling revisited)

Consider the general case of a system $\mathcal{S}$ interacting with a bath $\mathcal{B}$, described by the total hamiltonian

$$H_T = H_S + H_B + \lambda H_I. \quad (8)$$

The factor λ is a constant that serves to monitor the strength of the interaction between $\mathcal{S}$ and $\mathcal{B}$. The density matrix of the total system $\rho_T(t)$ obeys the exact unitary evolution:

$$\frac{d}{dt}\rho_T(t) = -i[H_T, \rho_T(t)] \quad (9)$$

Therefore we search some approximation to the dynamics of the reduced density matrix $\rho(t)$ of system $\mathcal{S}$

$$\rho(t) = \text{Tr}_B\left(e^{-itH_T}\rho(0)\otimes\rho_B^e e^{itH_T}\right) \quad (10)$$

Here $\rho_B^e = \rho_B(0)$ is the density matrix that describes the equilibrium state of the bath $\mathcal{B}$, and we have supposed that $\mathcal{S}$ and $\mathcal{B}$ were uncoupled before $t = 0$, so that $\rho_T(0) = \rho(0) \otimes \rho_B(0)$. The trace is taken over the bath variables, thereby reducing the evolution in the Hilbert space $\mathbf{H}_T = \mathbf{H}_S \otimes \mathbf{H}_B$ to an evolution in $\mathbf{H}_S$. Note that equation (10) defines a mapping of $\rho(0)$ onto $\rho(t)$, however this map is not a semigroup.

The Markov approximation can easily be introduced, in the interaction representation, by assuming: (i) that for all time the total density matrix factorize into a direct product; (ii) a perturbation theory to the differential equation of motion (9) up to order $\lambda^2\tau_c$ (τ_c is characterized by the highest correlation time of the operators of $\mathcal{B}$, which strongly depends on the nature of the bath); and (iii) that τ_c is sufficiently small such that $\tau_c \ll t$. Therefore the "quantum master equation" is obtained, *i.e.*, the semigroup approximation [1, 4, 8, 19–21].

$$\frac{d}{dt}\rho(t) = -i[H_S, \rho(t)] - \lambda^2\int_0^\infty d\tau \text{Tr}_B\left([H_I, [H_I(-\tau), \rho(t)\otimes\rho_B^e]]\right) \quad (11)$$

where $H_I(-\tau) \equiv e^{-i\tau(H_B+H_S)} H_I\, e^{i\tau(H_B+H_S)}$.

Remark 2. Equation (11) can be written in a K-L *form*. We emphasize that with the word *form* we are not saying that the *algebraic structure* is going to be positive, *i.e.*, only the hermitian condition on $a_{\alpha\gamma}$ is assured.

This fact follows by introducing the Jacobi identity

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$$

into the integrand of formula (11), then we get

$$\frac{d}{dt}\rho(t) = -i[H_S, \rho(t)] - \frac{\lambda^2}{2}\int_0^\infty d\tau \mathrm{Tr}_B \Big([[H_I, H_I(-\tau)], \rho(t)\otimes\rho_B^e] + [H_I, [H_I(-\tau), \rho(t)\otimes\rho_B^e]] + [H_I(-\tau), [H_I, \rho(t)\otimes\rho_B^e]] \Big) \quad (12)$$

Now, using that

$$[A,[B,C]] + [B,[A,C]] = \{\{A,B\}_+, C\}_+ - 2(ACB + BCA),$$

Equation (12) reduces to

$$\frac{d\rho(t)}{dt} = -i[H_{\mathrm{eff}}, \rho(t)] - \{D, \rho(t)\}_+ + F[\rho(t)], \quad (13)$$

with

$$H_{\mathrm{eff}} = H_S - i\frac{\lambda^2}{2}\int_0^\infty d\tau\, \mathrm{Tr}_B\Big([H_I, H_I(-\tau)]\,\rho_B^e\Big), \quad (14)$$

$$D = \frac{\lambda^2}{2}\int_0^\infty d\tau\, \mathrm{Tr}_B\Big(\{H_I, H_I(-\tau)\}_+\,\rho_B^e\Big), \quad (15)$$

$$F[\rho(t)] = \lambda^2\int_0^\infty d\tau\, \mathrm{Tr}_B\Big(H_I\,\rho(t)\otimes\rho_B^e\,H_I(-\tau) + H_I(-\tau)\,\rho(t)\otimes\rho_B^e\,H_I\Big). \quad (16)$$

Therefore (13) has the K-L *form*, to see this compare with Eq. (3).

Now to obtain the algebraic structure $a_{\alpha\gamma}$ we assume that the interaction hamiltonian H_I has the general expression

$$H_I = \sum_{\beta=1}^{n} V_\beta \otimes B_\beta, \qquad n \le N^2 - 1, \quad (17)$$

where the V_β belong to the Hilbert space of the finite dimensional system $\mathcal{S}$ and B_β are bath operators.

Using explicitly the fact that H_I is hermitian, (14) to (16) can be rewritten in a slightly different manner, this fact will be of utility for our future algebra. Introducing the notation

$$\chi_{\alpha\beta}(-\tau) \equiv \mathrm{Tr}_B\Big(\rho_B^e\, B_\alpha^\dagger\, B_\beta(-\tau)\Big) \quad (18)$$

in those equations, the effective Hamiltonian H_{eff}, the dissipative operator D and the fluctuating superoperator $F[\bullet]$ read

$$H_{\mathrm{eff}} = H_S - i\frac{\lambda^2}{2}\sum_{\alpha\beta}\int_0^\infty d\tau\Big(\chi_{\alpha\beta}(-\tau)V_\alpha^\dagger V_\beta(-\tau) - \chi_{\alpha\beta}^*(-\tau)V_\beta^\dagger(-\tau)V_\alpha\Big), \quad (19)$$

$$D = \frac{\lambda^2}{2}\sum_{\alpha\beta}\int_0^\infty d\tau\Big(\chi_{\alpha\beta}(-\tau)V_\alpha^\dagger V_\beta(-\tau) + \chi_{\alpha\beta}^*(-\tau)V_\beta^\dagger(-\tau)V_\alpha\Big), \quad (20)$$

$$F[\bullet] = \lambda^2\sum_{\alpha\beta}\int_0^\infty d\tau\Big(\chi_{\alpha\beta}(-\tau)V_\beta(-\tau)\bullet V_\alpha^\dagger + \chi_{\alpha\beta}^*(-\tau)V_\alpha\bullet V_\beta^\dagger(-\tau)\Big). \quad (21)$$

Finally, defining the matrix $C_{\beta\gamma}(-\tau)$ from

$$V_\beta(-\tau) \equiv e^{-i\tau H_S}V_\beta e^{+i\tau H_S} = \sum_{\gamma=1}^{N^2-1} C_{\beta\gamma}(-\tau)V_\gamma \quad (22)$$

and using the fact that the indices in (19) to (21) are dumb, Eq. (13) can be put as in the previous form (1)

$$\frac{d\rho(t)}{dt} = -i[H_{\mathrm{eff}}, \rho(t)] + \frac{1}{2}\sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma}\Big([V_\alpha, \rho(t)V_\gamma^\dagger] + [V_\alpha\rho(t), V_\gamma^\dagger]\Big), \quad (23)$$

where

$$H_{\mathrm{eff}} = H_S - i\frac{\lambda^2}{2}\sum_{\alpha\beta\gamma}\int_0^\infty d\tau\Big(\chi_{\gamma\beta}(-\tau)C_{\beta\alpha}(-\tau) - \chi_{\alpha\beta}^*(-\tau)C_{\beta\gamma}^*(-\tau)\Big)V_\gamma^\dagger V_\alpha, \quad (24)$$

and

$$a_{\alpha\gamma} = \lambda^2\sum_\beta\int_0^\infty d\tau\Big(\chi_{\gamma\beta}(-\tau)C_{\beta\alpha}(-\tau) + \chi_{\alpha\beta}^*(-\tau)C_{\beta\gamma}^*(-\tau)\Big). \quad (25)$$

Armed with these definitions we can now analyze the algebraic structure $a_{\alpha\gamma}$. From Eq. (25) it is simple to see that matrix $a_{\alpha\gamma}$ is hermitian. Nevertheless in order to arrive to a positive algebraic structure some restrictions on the interaction hamiltonian H_I must be introduced (see Sect. 4.1).

Remark 3. A necesary condition to assure that the algebraic structure will be *positive* can be seen in the following way. Let the half-Fourier transform of the correlations of the bath not to be cero; and let us assume that the interaction hamiltonian is written in a particular basis as $H_I =$

$\sum_{\beta=1}^{n} V_\beta \otimes B_\beta$ with $n \leq N^2 - 1$. Then the set $\{V_\beta\}_{\beta=1}^{n}$ ought to be closed under the Heisenberg representation, *i.e.*,

$$V_\beta(-\tau) \equiv e^{-i\tau H_S} V_\beta e^{+i\tau H_S} = \sum_{\gamma=1}^{m} C_{\beta\gamma}(-\tau) V_\gamma, \qquad \text{with} \quad m \leq n \tag{26}$$

otherwise the matrix $a_{\alpha\gamma}$ will not be positive.

When $m > n$ Sylvester's criterium shows that this affirmation can easily be proved by writing the elements of matrix (25). Note that if (26) is not fulfilled there will be (non-null) off-diagonal elements $a_{\alpha\gamma}$, and because the corresponding diagonal element is null this fact inevitably leads to the algebraic structure to be non-positive. A simple example is the Spin-Boson system with an interaction hamiltonian proportional to Pauli matrix σ_x. In this case condition (26) is not fulfilled, thus giving for this model a non-positive matrix $a_{\alpha\gamma}$.

Remark 4. Introducing the definition

$$\Gamma_{\alpha\beta}(-\tau) \equiv \mathrm{Tr}_B\left(\rho_B^e\, B_\alpha\, B_\beta(-\tau)\right) \tag{27}$$

in (14), the effective hamiltonian can also be written in the following way:

$$H_{\text{eff}} = H_S - i\frac{\lambda^2}{2}\sum_{\alpha\beta}\int_0^\infty d\tau \Big(\Gamma_{\alpha\beta}(-\tau)V_\alpha V_\beta(-\tau) - \Gamma^*_{\alpha\beta}(-\tau)V^\dagger_\beta(-\tau)V^\dagger_\alpha\Big) \tag{28}$$

using in this expression the matrix $C_{\beta\gamma}(-\tau)$ [see definition (22)] it results

$$H_{\text{eff}} = H_S - i\frac{\lambda^2}{2}\sum_{\alpha\beta\gamma}\int_0^\infty d\tau \Big(\Gamma_{\alpha\beta}(-\tau)C_{\beta\gamma}(-\tau)V_\alpha V_\gamma - \Gamma^*_{\alpha\beta}(-\tau)C^*_{\beta\gamma}(-\tau)V^\dagger_\gamma V^\dagger_\alpha\Big). \tag{29}$$

Note that it was possible to write expression (28) because the interaction hamiltonian is hermitian. Then the use of the *pseudo-correlation* $\Gamma_{\alpha\beta}(-\tau)$ is only a change of notation! These formulas will be seen of utility in order to compare with the Schrödinger-Langevin picture (see Sect. 5).

4. The Davies device

In the context of the trace-out technique it is well known that using Davies's averaging procedure the reduced dynamics turns to be a K–L semigroup [4, 6, 19], *i.e.*, the algebraic structure results always positive. In this section we want to explore the definitions of the dissipative operator D and the fluctuating superoperator $F[\bullet]$ from the point of view of the application of Davies's device. In general this mathematical device is defined by

$$K^\# = \lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}\exp\left(it\left[H_S,\bullet\right]\right) \times K\exp\left(-it\left[H_S,\bullet\right]\right)dt. \tag{30}$$

Here we have used the short notation $\exp\left(it\left[H_S,\bullet\right]\right)K \equiv e^{itH_S}Ke^{-itH_S}$.

Let us rewrite D and $F[\bullet]$ in terms of the operators Q_w defined by

$$V_\beta(-\tau) \equiv e^{-i\tau H_S}V_\beta e^{+i\tau H_S} = \sum_w Q_w^\beta e^{(-i\tau w)}$$

$$Q_w^\beta = \sum_{\varepsilon_n - \varepsilon_{n'} = w} \langle n| V_\beta |n'\rangle \; |n\rangle\,\langle n'|, \tag{31}$$

Note that here $\sum_{\varepsilon_n-\varepsilon_{n'}=w}$ means a sum over all n, n' under the constraint $w = \varepsilon_n - \varepsilon_{n'}$. Using the short notation (18), and (31) we can rewrite D, from (20), as

$$D = \frac{\lambda^2}{2}\sum_{\alpha,\beta,w,w'}\int_0^\infty d\tau\left(\chi_{\alpha\beta}(-\tau)e^{(-i\tau w')} + \chi^*_{\beta\alpha}(-\tau)e^{(i\tau w)}\right)Q_w^{\dagger\alpha}Q_{w'}^\beta. \tag{32}$$

In the same manner $F[\bullet]$, from (21), adopts the form:

$$F[\bullet] = \lambda^2\sum_{\alpha,\beta,w,w'}\int_0^\infty d\tau\left(\chi_{\alpha\beta}(-\tau)e^{(-i\tau w')} + \chi^*_{\beta\alpha}(-\tau)e^{(i\tau w)}\right)Q_{w'}^\beta \bullet Q_w^{\dagger\alpha}. \tag{33}$$

From these equations it is easy to see that after the application of Davies's device (30) all terms with different frequencies cancel out. Thus using the stationary property of the bath: $\chi_{\alpha\beta}(-\tau) = \chi^*_{\beta\alpha}(\tau)$, it is possible to obtain

$$D^\# = \frac{\lambda^2}{2}\sum_{\alpha,\beta,w}\int_{-\infty}^{\infty}d\tau\,\chi_{\alpha\beta}(-\tau)e^{(-i\tau w)}Q_w^{\dagger\alpha}Q_w^\beta, \tag{34}$$

$$F^\#[\bullet] = \lambda^2\sum_{\alpha,\beta,w}\int_{-\infty}^{\infty}d\tau\,\chi_{\alpha\beta}(-\tau)e^{(-i\tau w)}Q_w^\beta \bullet Q_w^{\dagger\alpha}. \tag{35}$$

From these expressions we immediately recognize the *algebraic structure* (compare with (5), (6)). The positivity of the *algebraic structure* follows from Bochner's theorem, because the matrix $\Xi_{\alpha\beta}(w) \equiv \int_{-\infty}^{\infty}d\tau\chi_{\alpha\beta}(-\tau)e^{(-i\tau w)}$ can be shown to be positive definite if $\chi_{\alpha\beta}(-\tau)$ represent the correlation functions of a thermal bath. Also note that $\chi_{\alpha\beta}(-\tau)$ fulfills KMS condition and this guarantees Detailed Balance for the generator (see appendix A.3, pag. 90, of Ref. 4).

If the spectrum of H_S is nondegenerate, it is straightforward to see that after Davies's device the diagonal elements of the density matrix evolve obeying a Pauli master equation, and the non-diagonal elements decay oscillating. The term giving rise to the gain in the Pauli master equation is $F^\#[\bullet]$.

To see this note that any diagonal element of (35) can be written in the form

$$\langle n \mid F^{\#}[\rho] \mid n\rangle = \lambda^2 \sum_{\alpha,\beta,w} \Xi_{\alpha\beta}(w) \times \sum_{l} \langle n \mid V_\beta \mid l\rangle \langle l \mid V_\alpha^\dagger \mid n\rangle \langle l \mid \rho \mid l\rangle \, \delta_{\varepsilon_n - \varepsilon_l, w}$$

which gives the well known Golden rule if we interchange the order of the sum $\sum_l$ with $\sum_w$ [19]. In addition, the lost term in the Pauli master equation comes from $-\left\{D^{\#}, \rho(t)\right\}_+$ in (13).

4.1. Invariance under Davies's device

Now the following question is in progress: Which are the types of interaction hamiltonians H_I that leave the superoperator $K[\bullet]$ invariant under Davies's device? Using (13) and due to the fact that it must be true for any density matrix it follows that $H_{\rm eff}$, D and $F[\bullet]$ ought to be invariant separately. It is possible to see that the invariance of $F[\bullet]$ implies the invariance of its dual $F^*[\bullet]$, thus using that $F^*[\mathbf{1}] = D$ the invariance of D is proved if $F[\bullet]$ is invariant. From this fact it is enough to demand the invariance of $F[\bullet]$ and $H_{\rm eff}$. Applying Davies's device to (16) we get

$$\begin{aligned} F^{\#}[\rho] &= \lambda^2 \lim_{\mathrm{T}\to\infty} \frac{1}{2\mathrm{T}} \int_{-\mathrm{T}}^{\mathrm{T}} dt \, e^{it[H_S,\bullet]} \int_0^\infty d\tau \mathrm{Tr}_B \left(H_I \, \rho \otimes \rho_B^e \; H_I(-\tau) + H_I(-\tau) \rho \otimes \rho_B^e \; H_I \right) e^{-it[H_S,\bullet]} \\ &= \lambda^2 \lim_{\mathrm{T}\to\infty} \frac{1}{2\mathrm{T}} \int_{-\mathrm{T}}^{\mathrm{T}} dt \int_0^\infty d\tau \mathrm{Tr}_B \left(H_I(t) \; \rho \otimes \rho_B^e \; H_I(t-\tau) + H_I(t-\tau) \; \rho \otimes \rho_B^e \; H_I(t) \right), \end{aligned} \tag{36}$$

where we have used that correlations $\mathrm{Tr}_B(\rho_B^e B_\alpha^\dagger B_\beta(-\tau))$ are stationary. Invariance of $F[\bullet]$ and $H_{\rm eff}$ under Davies's device means $F[\bullet] = F^{\#}[\bullet]$ and $H_{\rm eff} = H_{\rm eff}^{\#}$. Thus it is possible to see that both equalities are fulfilled if the following sufficient condition is held

$$\int_0^\infty d\tau \; \mathrm{Tr}_B \left(H_I(-\tau) \; \rho \otimes \rho_B^e H_I \right) = \int_0^\infty d\tau \; \mathrm{Tr}_B \left(\lim_{\mathrm{T}\to\infty} \frac{1}{2\mathrm{T}} \int_{-\mathrm{T}}^{\mathrm{T}} dt H_I(t-\tau) \; \rho \otimes \; \rho_B^e H_I(t) \right) \tag{37}$$

Note that the hermitian conjugate of (37) is also fulfilled, so the invariance of $H_{\rm eff}$ is guaranteed.

Equation (37) is the starting point to classify hamiltonians H_I which leave the generator $K[\bullet]$ invariant under Davies's average procedure.

The next step is to characterize condition (37) in a given particular basis using an interaction Hamiltonian of the form: $H_I = \sum_\beta V_\beta \otimes B_\beta$. In order to carry on this analysis, in this paper we will only be concerned with a spin-like Hmiltonian $H_S = \alpha \vec{S} \cdot \vec{B}_M$, where $\vec{S}$ is a vector operator (angular momentum of the system $\mathcal{S}$) and $\vec{B}_M$ is an external magnetic vector field. Therefore it is possible to interpret Davies's device as producing an average of the rotated operators in the Hilbert space $\mathbf{H}_S$, where the direction of this rotation is characterized by the external magnetic field $\vec{B}_M$ and the "angle" is the time. In this particular case it is always possible to find a basis in such a way that $H_S = \alpha S_z B_M$ so the rotation is along the z-axes. Taking advantage of this geometrical interpretation we choose to write the interaction Hamiltonian H_I in the basis of the irreducible spherical tensor operators of rank k [20]

$$H_I = \sum_{k=1}^{N-1} \sum_{q=-k}^{k} \mathrm{T}_k^q \otimes B_k^q \tag{38}$$

Here B_k^q are operators of the thermal bath $\mathcal{B}$ and T_k^q acts on $\mathbf{H}_S$. These operators fulfill the conditions (i) that they are traceless and orthogonal [basis in the C^* algebra of the $N\times N$ complex matrix $\mathcal{M}(N)$]; (ii) that they satisfy $\mathrm{T}_k^{-q} = \mathrm{T}_k^{\dagger q}$; and (iii) that if U_R is an unitary operator representing a rotation R then, $U_R \mathrm{T}_k^q U_R^\dagger = \sum_{q'=-k}^{k} \mathrm{T}_k^{q'} D_{q'q}^k$ where $D_{q'q}^k$ are the elements of the irreducible representation of the rotation group.

As we have remarked before we are interested in a rotation in the z-axes, thus

$$D_{q'q}^k = e^{-iq\theta} \delta_{qq'}.$$

So the irreducible spherical tensor operators, under a rotation along z- axes are only affected by a phase-shift that depends on q in the form

$$U_R \mathrm{T}_k^q U_R^\dagger = \mathrm{T}_k^q(-\theta) = e^{-iq\theta} \mathrm{T}_k^q. \tag{39}$$

Introducing (38) in the *rhs* of (37), and using (39) we arrive to

$$\int_0^\infty d\tau \lim_{\mathrm{T}\to\infty} \frac{1}{2\mathrm{T}} \int_{-\mathrm{T}}^{\mathrm{T}} dt \, \mathrm{Tr}_B \Big(\sum_{k,q} \sum_{k',q'} \mathrm{T}_{k'}^{q'}(t-\tau) \otimes B_{k'}^{q'}(t-\tau) \, (\rho \otimes \rho_B^e) \mathrm{T}_k^q(t) \otimes B_k^q(t) \Big)$$

$$= \sum_{k,q} \sum_{k',q'} \int_0^\infty d\tau \mathrm{Tr}_B \Big(\rho_B^e B_k^q \cdot B_{k'}^{q'}(-\tau) \Big) e^{-iq'\tau} \mathrm{T}_{k'}^{q'} \, \rho \, \mathrm{T}_k^q \lim_{\mathrm{T}\to\infty} \frac{1}{2\mathrm{T}} \int_{-\mathrm{T}}^{\mathrm{T}} dt \, e^{i(q+q')t}$$

$$= \sum_{k,k'} \sum_{q} \int_0^\infty d\tau \mathrm{Tr}_B \Big(\rho_B^e B_k^q \cdot B_{k'}^{-q}(-\tau) \Big) e^{iq\tau} \mathrm{T}_{k'}^{-q} \, \rho \, \mathrm{T}_k^q \tag{40}$$

Under these conditions [*i.e.*, $H_S = \alpha \vec{S} \cdot \vec{B}_M$, H_I given by (38), and the thermal bath fulfilling KMS condition] equation (37) means that if we want to have a superoperator $K[\bullet]$ which is invariant under Davies's device, a sufficient condition will be

$$\int_0^\infty d\tau \mathrm{Tr}_B \Big(\rho_B^e B_k^q \cdot B_{k'}^{q'}(-\tau) \Big) e^{-iq'\tau} = 0 \qquad \text{for} \quad q' \neq -q. \tag{41}$$

In this way the application of Davies's average will not produce any change in the dynamics of the reduced system, i.e. $K[\bullet] = K^{\#}[\bullet]$. A simple example where this condition is fulfilled is the Spin-Boson system with $H_S \propto \mathrm{T}_1^0$, $H_I = \sum_n \mathrm{T}_1^1 \otimes a_n + \mathrm{T}_1^{-1} \otimes a_n^\dagger$. Where $B_1^1 = \sum_n a_n$, $B_1^{-1} = \sum_n a_n^\dagger$, and a_n are boson operators of $\mathcal{B}$.

From condition (41) we note that the effect of Davies's average is to eliminate the terms in $F[\bullet]$ which do not have the symmetry under a rotation in the z direction, *i.e.* the same symmetry as H_S. Only in this form the invariance of the corresponding semigroup generator $K[\bullet]$ will be guaranteed. Condition (41) might be seen restrictive to a few interaction hamiltonians H_I, but we have found that this condition is a clear and plausible physical interpretation of what Davies's device produces.

5. The stochastic state vector approach

In this section we present an analysis concerning the so called Schrödinger-Langevin picture, their similarities and differences between other alternative stochastic formulations for quantum dissipative theories [1, 9–13, 15, 16]. In van Kampen's presentation [1], he was only concerned in getting the *standard* K-L generator, without looking at the effective hamiltonian (the shift) neither to the temperature-dependence on the algebraic structure. Latter on, in order to get the temperature-dependence in the algebraic structure $a_{\alpha\gamma}$, non-white noises were introduced in the approach [9].

We will show that from this formalism it is possible to obtain a quantum dissipative generator of the K-L *form* and we will show that in order to get a one-to-one correspondence with the *trace-out* technique, a light difference in the approach ought to be introduced. Also the numerical benefit—of the present approach—to get a *stochastic state vector* which corresponds to a thermal ensemble representing system $\mathcal{S}$ in contact with its environment, will be pointed out.

The starting point of the formalism, is to postulate a stochastic multiplicative equation for the state vector of the system $\mathcal{S}$ in contact with a thermal bath $\mathcal{B}$. This equation is written in terms of an unknown hermitian linear operator U, which is determined in a consistent way. The conservation in mean value of the norm of the wave function of the system $\mathcal{S}$, at any time, will be guarantee. The occurrence of a random operator $\mathcal{F}(t)$ in the Schrödinger-Langevin equation represents the effect of the interaction with the thermal bath $\mathcal{B}$. The Schrödinger-Langevin equation reads

$$\frac{d}{dt} |\Psi\rangle = \Big(-iH_S - \lambda [U + i\,\mathcal{F}(t)] \Big) |\Psi\rangle \tag{42}$$

and its adjoint

$$\frac{d}{dt} \langle\Psi| = \langle\Psi| \Big(iH_S - \lambda \big[U - i\,\mathcal{F}^\dagger(t)\big] \Big), \tag{43}$$

where λ is a coupling parameter, U is the hermitian linear operator to be determined later on, $\mathcal{F}(t)$ is an arbitrary stationary stochastic operator with $\langle \mathcal{F}(t) \rangle = 0$, and $\mathcal{F}^\dagger(t)$ represents its adjoint. In the present approach the dissipation and the fluctuations are both assumed to be of the same order in λ.

Introducing the *stochastic matrix* $\rho_{st}(t) \equiv |\Psi\rangle\langle\Psi|$ the connection between the reduced density matrix $\rho(t)$ and the wave function, in the Schrödinger-Langevin picture, is given by the assumption that in mean-value *over* the realizations of $\mathcal{F}(t)$ and $\mathcal{F}^\dagger(t)$

$$\rho(t) = \langle \rho_{st}(t) \rangle. \tag{44}$$

The probabilistic weight of each realization $\rho_{st}(t)$ is characterized by the probability of the corresponding realization of the matrix-noises. From (42) and (43) the stochastic matrix $\rho_{st}(t)$ evolves with the following non-Markovian equation

$$\frac{d}{dt}\rho_{st}(t) = -i[H_S, \rho_{st}(t)] - \lambda \{U, \rho_{st}(t)\}_+ - i\lambda \Big(\mathcal{F}(t)\,\rho_{st}(t) - \rho_{st}(t)\mathcal{F}^\dagger(t) \Big). \tag{45}$$

A clear interpretation of this evolution equation can be seen immediately as follows. Due to the fact that in general the stochastic operator $\mathcal{F}(t)$ is non-hermitian, it is possible to separate it in the form

$$\mathcal{F}(t) = \tilde{H}(t) - i\tilde{U}(t), \tag{46}$$

where $\tilde{H}(t)$ and $\tilde{U}(t)$ are stationary stochastic hermitian operators with cero mean value. Their expressions in terms of the operator $\mathcal{F}(t)$ are trivially given by

$$\tilde{H}(t) = \frac{1}{2}\Big(\mathcal{F}(t) + \mathcal{F}^{\dagger}(t)\Big),$$
$$\tilde{U}(t) = \frac{i}{2}\Big(\mathcal{F}(t) - \mathcal{F}^{\dagger}(t)\Big). \tag{47}$$

Introducing this notation in Eq. (42) the evolution of the *stochastic state vector* can be rewritten as

$$\frac{d}{dt}|\Psi\rangle = -i\left(H_S + \lambda\tilde{H}(t)\right)|\Psi\rangle - \lambda\left(U + \tilde{U}(t)\right)|\Psi\rangle. \tag{48}$$

Therefore each realization of the *stochastic matrix* $\rho_{st}(t)$ satisfies the non-Markovian evolution equation

$$\frac{d}{dt}\rho_{st}(t) = -i[H_S + \lambda\tilde{H}(t), \rho_{st}(t)] - \lambda\left\{U + \tilde{U}(t), \rho_{st}(t)\right\}_+, \tag{49}$$

which is nothing more than (45) rewritten in terms of hermitian operators. Now its physical interpretation is more clear, from (49) note that: (i) in von Neumann's term the total hamiltonian has a random fluctuating contribution $\lambda\tilde{H}(t)$. (ii) In the purely irreversible term (anti-commutator) there are two contributions: the first from the sure operator U and the second from the random operator $\tilde{U}(t)$ representing its fluctuations.

A remarkable point is that both random operators $\tilde{H}(t)$ and $\tilde{U}(t)$ are correlated, and this correlation will depend on the chosen interaction model between our system of interest and the bath. In general it can be temperature dependent.

In what follows, from (45) we will introduce a second-order perturbation theory in the coupling parameter λ, see Subsect. 5.1. In order to get a closed equation for the reduced density matrix $\langle\rho_{st}(t)\rangle$ of $\mathcal{S}$, the unknown operator U will be found in a consistent way demanding $\mathrm{Tr}\,\langle\rho_{st}(t)\rangle = 1$, then the linear (sure) operator U will result characterized by the correlations of the stochastic operators $\mathcal{F}(t)$ and $\mathcal{F}^{\dagger}(t)$.

In the next subsections we will analyze several possibilities that come from the different elections for the random operator $\mathcal{F}(t)$. In Subsect. 5.2 we will present the hermitian case, *i.e.*, when $\mathcal{F}(t) = \mathcal{F}^{\dagger}(t)$. In this situation a stochastic hamiltonian evolution, for the *stochastic state vector*, will result. As we are going to show, in this case, the dissipation into the reduced density matrix comes from the second cumulant of $\tilde{H}(t)$. In this particular case each realization of the *stochastic state vector* is normalized, and the correspondence with the infinite temperature approximation will be pointed out [22]. In Subsect. 5.3 we will present the anti-hermitian case, *i.e.*, $\mathcal{F}(t) = -\mathcal{F}^{\dagger}(t)$. In this situation only the average of the *stochastic state vector* is normalized. In Subsect. 5.4 we will present the full non-hermitian case, *i.e.*, $\mathcal{F}(t) \neq \mathcal{F}^{\dagger}(t)$. As we will show, for this particular case, the evolution equation of the reduced density matrix can be mapped with the (dissipative) dynamics that comes from the tracing-out techniques. Thus we will prove the equivalence of its corresponding K-L *form* with the one obtained in our previous sections [17]. In Subsect. 5.5 some advantages on the present stochastic picture are pointed out.

5.1. The second-order cumulant approximation

The Eq. (45) is a stochastic multiplicative operational equation (in general with non-white noise). The most general stochastic Eq. (45), with an arbitrary multiplicative noise, can be written in the compact form

$$\frac{d}{dt}u(t) = [A_o + \lambda\, A_1(t)]\, u(t), \tag{50}$$

where A_o is a deterministic superoperator and $A_1(t)$ is a stochastic one characterized by its statistical properties. Using Stratonovich's calculus in a second-order cumulant expansion [1] (in the small Kubo number $\lambda\tau_c$) and assuming that the correlation time τ_c of the stochastic operator $A_1(t)$ is smaller than any deterministic evolution time of $u(t)$, the average $\langle u(t)\rangle$ satisfies the closed Markovian equation

$$\frac{d}{dt}\langle u(t)\rangle = \left(A_o + \lambda\,\langle A_1(t)\rangle + \lambda^2\int_0^{\infty} d\tau\,\langle\langle A_1(t)\,e^{\tau A_o} A_1(t-\tau)\rangle\rangle\, e^{-\tau A_o}\right)\langle u(t)\rangle \tag{51}$$

Then we can identify

$$\langle u(t)\rangle \equiv \langle\rho_{st}(t)\rangle = \rho(t), \qquad A_o \equiv -i[H_s, \bullet], \qquad A_1(t) \equiv -\{U, \bullet\}_+ - i\left(\mathcal{F}(t)\bullet - \bullet\,\mathcal{F}^{\dagger}(t)\right). \tag{52}$$

The second cumulant appearing in (51) is given by

$$\langle\langle A_1(t)\, e^{\tau A_o} A_1(t-\tau)\rangle\rangle e^{-\tau A_o} = \langle\langle\mathcal{F}(t)\bullet\mathcal{F}^{\dagger}\cdot(t-\tau)\rangle\rangle + \langle\langle\mathcal{F}(t-\tau)\bullet\mathcal{F}^{\dagger}(t)\rangle\rangle - \langle\langle\mathcal{F}(t)\,\mathcal{F}(t-\tau)\rangle\rangle\bullet - \bullet\,\langle\langle\mathcal{F}^{\dagger}(t-\tau)\,\mathcal{F}^{\dagger}(t)\rangle\rangle \tag{53}$$

All time-dependent operators are given in the Heisenberg representation, *i.e.*, $\mathcal{F}(\tau) \equiv e^{i\tau H_S}\mathcal{F}e^{-i\tau H_S}$. Thus (51) can be rewritten in the form

$$\frac{d}{dt}\rho(t) = -i[H_S, \rho(t)] - \lambda\{U, \rho(t)\}_+ + \lambda^2 \int_0^\infty \Big(\langle\!\langle \mathcal{F}(t)\rho(t)\mathcal{F}^\dagger(t-\tau)\rangle\!\rangle + \langle\!\langle \mathcal{F}(t-\tau)\rho(t)\mathcal{F}^\dagger(t)\rangle\!\rangle - \langle\!\langle \mathcal{F}(t)\mathcal{F}(t-\tau)\rangle\!\rangle \rho(t) - \rho(t)\langle\!\langle \mathcal{F}^\dagger(t-\tau)\mathcal{F}^\dagger(t)\rangle\!\rangle \Big) d\tau. \quad (54)$$

Demanding the condition $\mathrm{Tr}\rho(t) = 1$, the linear operator U must fulfill

$$U = \frac{\lambda}{2}\int_0^\infty d\tau \Big(\langle\!\langle \mathcal{F}^\dagger(t)\mathcal{F}(t-\tau)\rangle\!\rangle + \langle\!\langle \mathcal{F}^\dagger(t-\tau)\mathcal{F}(t)\rangle\!\rangle - \langle\!\langle \mathcal{F}(t)\mathcal{F}(t-\tau)\rangle\!\rangle - \langle\!\langle \mathcal{F}^\dagger(t-\tau)\mathcal{F}^\dagger(t)\rangle\!\rangle \Big). \quad (55)$$

In this manner the conservation in mean value of the stochatic wave function norm is guaranteed too[c]. Introducing the expression of U back in (54) and after a little of algebra the evolution of $\rho(t)$ can be written in the form

$$\frac{d\rho(t)}{dt} = -i[H_{\text{eff}}, \rho(t)] - \{D, \rho(t)\}_+ + F[\rho(t)], \quad (56)$$

where the hamiltonian shift is characterized by the effective Hamiltonian

$$H_{\text{eff}} = H_S - i\frac{\lambda^2}{2}\int_0^\infty d\tau \Big(\langle\!\langle \mathcal{F}(t)\mathcal{F}(t-\tau)\rangle\!\rangle - \langle\!\langle \mathcal{F}^\dagger(t-\tau)\mathcal{F}^\dagger(t)\rangle\!\rangle \Big) \quad (57)$$

The operator D and the superoperator $F[\bullet]$ are given by

$$D = \frac{\lambda^2}{2}\int_0^\infty d\tau \Big(\langle\!\langle \mathcal{F}^\dagger(t)\mathcal{F}(t-\tau)\rangle\!\rangle + \langle\!\langle \mathcal{F}^\dagger(t-\tau)\mathcal{F}(t)\rangle\!\rangle \Big) \quad (58)$$

$$F[\bullet] = \lambda^2 \int_0^\infty d\tau \Big(\langle\!\langle \mathcal{F}(t)\bullet\mathcal{F}^\dagger(t-\tau)\rangle\!\rangle + \langle\!\langle \mathcal{F}(t-\tau)\bullet\mathcal{F}^\dagger(t)\rangle\!\rangle \Big). \quad (59)$$

These equations show that the Schrödinger-Langevin picture leads to an evolution equation for $\rho(t)$ that has the form of a K-L generator (see Sect. 1). Thus we can get profit from the Schrödinger-Langevin picture by modeling different objects $\langle\!\langle \mathcal{F}^\dagger(t)\ \mathcal{F}(t-\tau)\rangle\!\rangle$. The positivity or not of its corresponding algebraic structure is something that strongly depends on the correlations $\langle\!\langle \mathcal{F}^\dagger(t)\ \mathcal{F}(t-\tau)\rangle\!\rangle$.

We point out that it is always possible to rewrite the last expressions for H_{eff}, D and $F[\bullet]$ in terms of the hermitian stochastic operators $\tilde{H}(t)$ and $\tilde{U}(t)$, see appendix B. The extension of this formalism to a higher order cumulant expansion is also shown in Appendix C.

5.2. Case when $\mathcal{F}(t)$ is a hermitian random operator

In this section we will assume that the random operator $\mathcal{F}(t)$, appearing in the Schrödinger-Langevin picture (42), is hermitian and we will search for its consequences. Using (46) it is trivial to see that if $\mathcal{F}(t) = \mathcal{F}^\dagger(t)$ it will be equivalent to $\mathcal{F}(t) = \tilde{H}(t)$ and $\tilde{U}(t) = 0$. On the other hand, from (55) it is simple to see that $U = 0$. Therefore from (48) and (49) the dynamics result

$$\frac{d}{dt}|\Psi\rangle = -i\Big(H_S + \lambda\tilde{H}(t)\Big)|\Psi\rangle, \quad (60)$$

and for the *stochastic matrix* $\rho_{st}(t)$

$$\frac{d}{dt}\rho_{st}(t) = -i[H_S + \lambda\tilde{H}(t), \rho_{st}(t)]. \quad (61)$$

We see that each realization of the *stochastic matrix* $\rho_{st}(t)$ is normalized as is, of course, the *stochastic state vector*. The remarkable point is that this type of evolution, stochastic Hamiltonian, give rise to a K-L *form.* Before going into any detail let us write H_{eff}, D, and $F[\bullet]$ in terms of the stochastic hamiltonian $\tilde{H}(t)$. Then Eqs. (57), (58) and (59) will read

$i)$ the effective Hamiltonian

$$H_{\text{eff}} = H_S - i\frac{\lambda^2}{2}\int_0^\infty d\tau\, \langle\!\langle [\tilde{H}(t), \tilde{H}(t-\tau)] \rangle\!\rangle; \quad (62)$$

$ii)$ the operator D

$$D = \frac{\lambda^2}{2}\int_0^\infty d\tau \langle\!\langle \{\tilde{H}(t), \tilde{H}(t-\tau)\}_+ \rangle\!\rangle; \quad (63)$$

$iii)$ the superoperator $F[\bullet]$

$$F[\bullet] = \lambda^2\int_0^\infty d\tau \Big(\langle\!\langle \tilde{H}(t)\bullet\tilde{H}(t-\tau)\rangle\!\rangle + \langle\!\langle \tilde{H}(t-\tau)\bullet\tilde{H}(t)\rangle\!\rangle \Big). \quad (64)$$

Note that in this case the Schrödinger-Langevin picture is formally equivalent to *trace-out* technique just by replacing $H_I \to \tilde{H}(t) = \tilde{H}(t)^\dagger$, see (14), (15), (16) and changing $\mathrm{Tr}[\bullet]$ by a second cumulant object.

What we will do now is to study which are the consequences if we assume that the stochastic hermitian operator $\mathcal{F}(t)$ were written as a linear combinations of complex-random numbers times operators in the Hilbert space of $\mathcal{S}$. This model is rather simpler than the one introduced by Fox [10] because in the present case only a cumulant theory of stochastic process is required. In that mentioned reference a highly complex matrix-cumulant theory had to be used to go ahead with a second-order perturbation; and in particular a boson bath was used to obtain the temperature dependence in the generator.

Therefore let us analyze the case when $\mathcal{F}(t)$ is hermitian, then it is characterized by

$$\mathcal{F}(t) = \tilde{H}(t) = \sum_{\alpha=1}^{n} l_\alpha(t) V_\alpha, \qquad n \leq N^2 - 1. \tag{65}$$

The complex numbers $l_\alpha(t)$ are in general stationary complex stochastic processes with mean value cero and non-white correlations. Owing to the hermiticity of $\tilde{H}(t)$ it follows that if $l_\alpha(t)$ were complex-numbers there will be an index α' such that $l_{\alpha'}(t)$ must be the complex-conjugated of $l_\alpha(t)$ ($V_{\alpha'} = V_\alpha^\dagger$), *i.e.*, $l_{\alpha'}(t) = l_\alpha^*(t)$ otherwise $\tilde{H}(t)$ would not be hermitian. Note that in the particular case when the operators V_α are hermitian the noises $l_\alpha(t)$ ought to be real.

Introducing this $\tilde{H}(t)$ in (62), (63) and (64) it is possible to see that the expressions for H_{eff}, D, and $F[\bullet]$ are formally the same as the one obtained from tracing-out in quantum mechanics, see (19), (20) and (21). In order to realize this fact the quantum correlations [see (18)] ought to be replaced by stationary noise correlations

$$\chi_{\alpha\beta}(-\tau) \rightarrow \langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle. \tag{66}$$

At this stage the correlations of the noises can be selected, in an empirical way, to represent different physical situations. For example, if the correlations of the noises were white [from (19) or (57)] it is simple to see that the shift cancel-out and the dissipative generator gives the *standard* K-L semigroup. Therefore a shift can only be obtained if the underlying dynamics is non-markovian.

Now we wonder if it is possible to find a complex stochastic process in such a way to match with the corresponding correlation functions that come from the operators of the bath B_α, see (18). Then these noises should satisfy

$$\mathrm{Tr}_B\left(\rho_B^e\, B_\alpha^\dagger\, B_\beta(-\tau)\right) \stackrel{?}{=} \langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle. \tag{67}$$

If this is the case we would have found an algebraic structure, from the Schrödinger-Langevin picture, which will be numerically equal to that $a_{\alpha\gamma}$ obtained from the trace-out technique. In what follows we will show that this is not possible to do. This is the main point why we will go, in the next sections, to the case when $\mathcal{F}(t)$ is non-hermitian.

Because $\tilde{H}(t)$ is hermitian we could make the correspondence $H_I \rightarrow \tilde{H}(t)$, then from (65) and (17) it is possible to assign to each operator of the bath a classical noise in the form

$$B_\alpha \rightarrow l_\alpha, \qquad B_\alpha^\dagger \rightarrow l_\alpha^*. \tag{68}$$

But this correspondence shows that it is not possible to reconcile both algebraic structures, as will be show by the following steps. In order to show this fact we use rule (68) in the following cases:

$$\chi_{\alpha\beta}(-\tau) \equiv \mathrm{Tr}_B\left(\rho_B^e\, B_\alpha^\dagger\, B_\beta(-\tau)\right) \longleftrightarrow \langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle,$$

$$\chi_{\alpha'\beta'}^*(-\tau) \equiv \mathrm{Tr}_B\left(\rho_B^e B_\beta(-\tau) B_\alpha^\dagger\right) \longleftrightarrow \langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle, \tag{69}$$

where we have used that $B_{\alpha'} = B_\alpha^\dagger$, $B_{\beta'} = B_\beta^\dagger$. From the *rhs* of (69) this mapping would be consistent, from the quantum point of view, if and only if

$$\chi_{\alpha\beta}(-\tau) = \chi_{\alpha'\beta'}^*(-\tau) \tag{70}$$

this means that

$$\mathrm{Tr}_B\left(\rho_B^e\, B_\alpha^\dagger\, B_\beta(-\tau)\right) = \mathrm{Tr}_B\left(\rho_B^e\, B_\beta(-\tau) B_\alpha^\dagger\right). \tag{71}$$

But in general this condition is not true because the bath operators do not commute. Therefore due to the non-commutativity of the bath operators an inconsistency to calculate the correlation functions $\langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle$ results from assignation (68).

In short, in the weak coupling approximation the random hamiltonian approach [complex-random numbers times operators in $\mathbf{H}_S$, whose generator is characterized by (62) to (64)], cannot provide a one-to-one mapping with the method of tracing-out the quantum bath variables. Only at infinite temperature [where $\rho_B^e \equiv e^{-\beta H_B}/\mathrm{Tr}[e^{-\beta H_B}]$ is the identity operator in the Hilbert space of the bath] condition (71) could be satisfied. Then, *only* at infinite temperature the random hamiltonian approach, with $\tilde{H}(t) = \sum_{\alpha=1}^{n} l_\alpha(t) V_\alpha$, would give exactly the same result as the one obtained from tracing-out techniques $\left(\text{with } H_I = \sum_{\alpha=1}^{n} V_\alpha \otimes B_\alpha\right)$. We emphasize that the same conclusion was already found by Abragam in the context of nuclear magnetism [22].

5.3. Case when $\mathcal{F}(t)$ is a anti-hermitian random operator

In this section we will assume that the random operator $\mathcal{F}(t)$ is anti-hermitian. Using (46) it is trivial to see that if $\mathcal{F}(t) = -\mathcal{F}^\dagger(t)$ it will be equivalent to $\mathcal{F}(t) = -i\tilde{U}(t)$ and $\tilde{H}(t) = 0$. Therefore the evolution is given by

$$\frac{d}{dt}|\Psi\rangle = -iH_S|\Psi\rangle - \lambda\left(U + \tilde{U}(t)\right)|\Psi\rangle. \tag{72}$$

Each realization of the *stochastic matrix* $\rho_{st}(t)$ satisfies

$$\frac{d}{dt}\rho_{st}(t) = -i[H_S, \rho_{st}(t)] - \lambda\left\{U + \tilde{U}(t), \rho_{st}(t)\right\}_+. \tag{73}$$

Is simple to see that the generator obtained (see appendix B) is the same that in the hermitian case making the following changes: $\tilde{H}(t) \to \tilde{U}(t)$ and changing the sign of the contribution to H_{eff}. If we asume that

$$i\mathcal{F}(t) = \tilde{U}(t) = \sum_{\alpha=1}^{n} l_\alpha(t) V_\alpha, \qquad n \le N^2 - 1, \qquad (74)$$

and again we try to match with the trace-out technique, the same problems that in the hermitian case are found. That is, a correlation map cannot be established consistently owing to the asignation (68). This one-to-one correspondence is now result of being $\tilde{U}(t)$ hermitian. As in the hermitian case, if the correlations of the noises were white, the shift cancel-out and the dissipative generator gives the *standard* K-L semigroup

In the next section we are going to analyze the most general case of the Schrödinger-Langevin evolution.

5.4. Case when $\mathcal{F}(t)$ is a non-hermitian random operator

Let us now analyze the case when $\mathcal{F}(t)$ is non-hermitian (nor anti-hermitian). This corresponds to the most general situation in the context of the Schrödinger-Langevin picture. As before let us assume that $\mathcal{F}(t)$ is a linear combination of stationary complex stochastic processes times operator in the Hilbert space of $\mathcal{S}$, then

$$\mathcal{F}(t) = \sum_{\alpha=1}^{n} l_\alpha(t) V_\alpha, \qquad n \le N^2 - 1. \qquad (75)$$

In this case we do not impose any restriction on $l_\alpha(t)$ as in previous sections due to the hermiticity (or anti-hermiticity) of $\mathcal{F}(t)$. Introducing (75) into the formulas (57), (58) and (59) we can see that the resulting expressions for H_{eff}, D, and $F[\bullet]$ are formally the same as the one obtained from tracing-out the bath variables, see (28), (20) and (21). From these results we emphasize that the same expression (as from quantum mechanics) for the algebraic structure $a_{\alpha\gamma}$ is obtained. In order to realize this fact the quantum correlations [see (18) and (27)] ought to be replaced by the stationary classical correlations of the noises:

$$\begin{aligned} \chi_{\alpha\beta}(-\tau) &\to \langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle, \\ \Gamma_{\alpha\beta}(-\tau) &\to \langle\langle l_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle. \end{aligned} \qquad (76)$$

Contrary to what happens by tracing-out and also in the case when $\mathcal{F}(t)$ is hermitian (or anti-hermitian, see previous section), here in the full non-hermitian case, $\mathcal{F}(t) \neq \mathcal{F}^\dagger(t)$, the pseudo-correlations $\langle\langle l_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle$ necessarily appear in the theory, *i.e.*, the generator (56) cannot be expressed in terms of $\langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle$ alone.

As before it is possible to choose different correlation functions in order to build up several K-L generators. The positivity of the algebraic structure strongly depends on the correlations $\langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle$. The pseudo-correlations only appear in the expression of H_{eff}.

Therefore, we have a total freedom to choose the correlation function of the noises as a possible empirical way to map different physical conditions. A simplest example is to assume that

$$\begin{aligned} \langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle &= \delta_{\alpha\beta}\,\delta(\tau), \\ \langle\langle l_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle &= 0. \end{aligned} \qquad (77)$$

In this particular case [uncorrelated white noises] from (55) we get $U = \frac{1}{2}\sum_\alpha V_\alpha^\dagger V_\alpha$ ($\lambda = 1$). Thus reobtaining van Kampen's approach [1], from which the *standard* K-L generator is obtained:

$$\dot{\rho}(t) = -i[H_S, \rho] - \frac{1}{2}\Big\{\sum_\alpha V_\alpha^\dagger V_\alpha, \rho\Big\}_+ + \sum_\alpha V_\alpha \rho V_\alpha^\dagger. \qquad (78)$$

This type of evolution equation was also analyzed by Ghirardi *et al.* [11] in the context of the wave-packet reduction approach.

In short, once again we ask for the problem of finding noises $l_\alpha(t)$ in such a way that $a_{\alpha\gamma}$ and H_{eff} be numerically equal to those coming from the tracing-out technique. Now due to the fact that we have a freedom for the election of the noise correlations, this issue will allow us to get a consistent *correlation mapping*.

To do this program let us start analyzing the dissipative part. Assume the that we have found noises such that the following equality is true

$$\mathrm{Tr}_B\left(\rho_B^e\, B_\alpha^\dagger\, B_\beta(-\tau)\right) \stackrel{?}{=} \langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle \qquad (79)$$

Now we can show that there is no inconsistency in the present correlation mapping, (that was not the case when $\mathcal{F}(t)$ was hermitian or anti-hermitian).

In order to see if there is some contradiction in the assignation rule (79) we now proceed to do the same steps that we made in the previous case. As before, because $H_I^\dagger \equiv H_I$, there exist an α' and β' such that: $B_{\alpha'} = B_\alpha^\dagger$, $B_{\beta'} = B_\beta^\dagger$; then from (79) it follows:

$$\begin{aligned} \chi_{\alpha\beta}(-\tau) &\equiv \mathrm{Tr}_B\left[\rho_B^e B_\alpha^\dagger\, B_\beta(-\tau)\right] \\ &\longleftrightarrow \langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle \\ \chi_{\alpha'\beta'}^*(-\tau) &\equiv \mathrm{Tr}_B\left(\rho_B^e B_\beta(-\tau) B_\alpha^\dagger\right) \\ &\longleftrightarrow \langle\langle l_{\alpha'}(t)\, l_{\beta'}^*(t-\tau)\rangle\rangle \end{aligned} \qquad (80)$$

But because[d] $l_{\alpha'}(t) \neq l_\alpha^*(t)$ and $l_{\beta'}(t) \neq l_\beta^*(t)$ there is no inconsistency in (80). In other words, this is so because in the present case it is not possible to establish a one-to-one mapping between bath operators B_α and complex noises $l_\alpha(t)$. Thus the fact that $\mathcal{F}(t) \neq \mathcal{F}^\dagger(t)$ gives us the freedom to find noises giving a consistent *correlation mapping*.

We remark that for the noise correlations $\langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle$, there are in fact four functions corresponding to the cross-correlations between the real and imaginary parts of the noises $l_\alpha(t)$, then (79) gives only two equations to determine these four real correlations. This fact gives us two (free) degrees of freedom in the choice of the complex-noises. Note that $\chi^*_{\alpha\beta}(-\tau)$ trivially does not introduce any new restriction, and on the other hand the stationary property $\chi_{\beta\alpha}(-\tau) = \chi^*_{\alpha\beta}(\tau)$ indicates that the corresponding (79) for $\chi_{\beta\alpha}(-\tau)$ does not impose any new restriction in the four real correlations necessary to build $\langle\langle l^*_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle$. In conclusion, we arrive to the same dissipative K-L *form* that was obtained from the tracing-out technique and without any inconsistency in the assignation rule (79).

Now we proceed to check if there is some contradiction to try to match with the non-dissipative part of the generator, *i.e.*, we now look if H_{eff} (obtained from Schrödinger-Langevin) is numerically the same as the one coming from the tracing-out. This task can be tackle because we still have two degree freedom to try to establish the following equality

$$\mathrm{Tr}_B\left(\rho^e_B\, B_\alpha\, B_\beta(-\tau)\right) \stackrel{?}{=} \langle\langle l_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle. \tag{81}$$

Even when this formula only introduces two new restrictions, these are inconsistent with the previous ones (79). To proof this fact note that because the interaction hamiltonian H_I is hermitian, there always exist an α' such that $B_{\alpha'} = B^\dagger_\alpha$, $V_{\alpha'} = V^\dagger_\alpha$. Then from the quantum point of view it is true that

$$\begin{aligned}\Gamma_{\alpha'\beta}(-\tau) &= \chi_{\alpha\beta}(-\tau) = \mathrm{Tr}_B\left(\rho^e_B\, B^\dagger_\alpha\, B_\beta(-\tau)\right),\\ \Gamma_{\alpha\beta}(-\tau) &= \chi_{\alpha'\beta}(-\tau) = \mathrm{Tr}_B\left(\rho^e_B\, B_\alpha\, B_\beta(-\tau)\right),\end{aligned} \tag{82}$$

and this must be true for all couples (α,α') appearing in H_I. Therefore from (81) it follows that noise correlations should fulfill

$$\begin{aligned}\langle\langle l_{\alpha'}(t)\, l_\beta(t-\tau)\rangle\rangle &= \langle\langle l^*_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle,\\ \langle\langle l_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle &= \langle\langle l^*_{\alpha'}(t)\, l_\beta(t-\tau)\rangle\rangle.\end{aligned} \tag{83}$$

From this equations it is possible to see that for all couples (α, α') appearing in H_I, it must be true that

$$l_{\alpha'}(t) = l^*_\alpha(t) \tag{84}$$

If this is so $\mathcal{F}(t)$ would be hermitian, but the hermitian case only matches the dissipative part from the trace-out technique at infinite temperature, and as a matter of fact this is not the case of interest in the present section. Therefore in order not to get any inconsistency from (81) we have to resign to match both, simultaneously, the irreversible and reversible part of the generator.

Therefore the two degrees of freedom are still undetermined. The remarkable point is that we can use this freedom to choose $\langle\langle l_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle = 0$. Then the resulting final *correlation-map* is

$$\begin{aligned}\chi_{\alpha\beta}(-\tau) \equiv \mathrm{Tr}_B\left(\rho^e_B\, B^\dagger_\alpha\, B_\beta(-\tau)\right) &= \langle\langle l^*_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle,\\ \langle\langle l_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle &= 0.\end{aligned} \tag{85}$$

In this way the *correlation-mapping*—for the Schrödinger-Langevin picture—will reproduce exactly the same dissipative part as is obtained from tracing-out techniques.

We emphasize that with this assignation rule and from (57), the shift coming from the Schrödinger-Langevin picture is null, then $H_{\text{eff}} = H_S$ and also from (55) and (58) it follows the identity

$$\lambda U = D \tag{86}$$

Then, the Schrödinger-Langevin picture results in

$$\frac{d}{dt}|\Psi\rangle = \Big(-iH_S - D - i\lambda\mathcal{F}(t)\Big)|\Psi\rangle \tag{87}$$

which means that the stochastic matrix $\rho_{st}(t)$ evolves with the following non-Markovian equation

$$\begin{aligned}\frac{d}{dt}\rho_{st}(t) = -i[H_S, \rho_{st}(t)] - \{D, \rho_{st}(t)\}_+\\ - i\lambda\Big(\mathcal{F}(t)\,\rho_{st}(t) - \rho_{st}(t)\mathcal{F}^\dagger(t)\Big)\end{aligned} \tag{88}$$

Then from (88) we can see, in the weak coupling approximation, that $\lambda U = D$ is the responsible of the dissipation and $\mathcal{F}(t)$ is the one producing the fluctuating terms $F[\bullet]$ in the K-L *form*. We remark that the positivity or not of the algebraic structure is something that depends on the structure of the interaction hamiltonian (see our previous section on the invariance under Davies's device).

5.5. Other possible applications

Let us now see other advantages from the Schrödinger-Langevin picture. Assume that we already have a given algebraic structure $a_{\alpha\gamma}$, (*i.e.*, a $M \times M$ positive hermitian matrix where $M = N^2 - 1$) then (25) can be seen in the reverse sense, *i.e.*, as a set of $\frac{1}{2}M(M+1)$ equations for the unknown noise correlations

$$\begin{aligned}a_{\alpha\gamma} = \lambda^2 \sum_\beta \int_0^\infty d\tau \Big(\langle\langle l^*_\gamma(t)\, l_\beta(t-\tau)\rangle\rangle C_{\beta\alpha}(-\tau)\\ + \langle\langle l_\alpha(t)\, l^*_\beta(t-\tau)\rangle\rangle C^*_{\beta\gamma}(-\tau)\Big).\end{aligned} \tag{89}$$

Note that all what we have made in previous sections was in fact to solve this non-trivial problem. But due to the fact that from the Schrödinger-Langevin picture its algebraic structure is formally the same as the one from tracing-out the bath variables, in that particular case these numerical equalities were just solved by making the correlation mapping that we have presented. Therefore we can conclude that we have provided a *non-Markovian evolution* corresponding to an open quantum system (where all effects of the bath are introduced through the correlations of the noises) that in the markovian approximation correspond to trace-out technique. This fact open the possibility of work out with non-Markovian simulations of the state vector.

When this case is not available and assuming that we have found a basis where the given $a_{\alpha\gamma}$ is diagonal, the resulting equations are

$$a_{\alpha\alpha} = \lambda^2 \sum_{\beta} \int_0^{\infty} d\tau \Big(\langle\langle l_{\alpha}^{*}(t)\, l_{\beta}(t-\tau)\rangle\rangle C_{\beta\alpha}(-\tau) + \langle\langle l_{\alpha}(t)\, l_{\beta}^{*}(t-\tau)\rangle\rangle C_{\beta\alpha}^{*}(-\tau) \Big) \quad (90)$$

and for the case $\alpha \neq \gamma$ results

$$0 = \sum_{\beta} \int_0^{\infty} d\tau \Big(\langle\langle l_{\gamma}^{*}(t)\, l_{\beta}(t-\tau)\rangle\rangle C_{\beta\alpha}(-\tau) + \langle\langle l_{\alpha}(t)\, l_{\beta}^{*}(t-\tau)\rangle\rangle C_{\beta\gamma}^{*}(-\tau) \Big). \quad (91)$$

If in addition the noises are assumed to be statistically independent from each other, using (90) and (91) we arrive to a simpler set of equations for the unknown noise correlations

$$a_{\alpha\alpha} = \lambda^2 \int_0^{\infty} d\tau \,\mathrm{Re}\, \Big(\langle\langle l_{\alpha}^{*}(t)\, l_{\alpha}(t-\tau)\rangle\rangle C_{\alpha\alpha}(-\tau) \Big), \quad (92)$$

and for $\alpha \neq \gamma$

$$0 = \int_0^{\infty} d\tau \Big(\langle\langle l_{\gamma}^{*}(t)\, l_{\gamma}(t-\tau)\rangle\rangle C_{\gamma\alpha}(-\tau) + \langle\langle l_{\alpha}(t)\, l_{\alpha}^{*}(t-\tau)\rangle\rangle C_{\alpha\gamma}^{*}(-\tau) \Big) \quad (93)$$

which are equations for the half-Fourier transform of the correlations. We emphasize that it is always possible to find a family of noises that satisfy these equations. This fact is shown elsewhere [17].

Therefore the advantage from our stochastic picture comes from a numerical point of view. This is so because solving non-equilibrium thermal statistical averages in the context of the *stochastic state vector* reduces the computational time in comparison with the one required by using density matrix algorithm.

We want to end this section remarking that the present stochastic picture leads to a numerical linear problem, with an easy interpretation.

6. Conclusions

The quantum generator of the semigroup has been written in an alternative form in terms of the dissipative operator D and the fluctuating superoperator $F[\bullet]$ [see (3) and also appendix A]. From the formal solution of the quantum semigroup, we have shown that D ought to be positive in order to erase the initial condition $\rho(t_o)$.

We have proved that a Kossakowki-Lindblad *form* is always obtained if we *trace-out* the bath variables of the total system $\mathcal{S} + \mathcal{B}$ [in a second-order perturbation theory applied to the differential form of the equation of motion, see (13) in *remark 2*]. Nevertheless we have remarked that a Kossakowki-Lindblad *form* does not mean that the *algebraic structure* $a_{\alpha\gamma}$ is going to be positive, this is something that concerns to the type of interaction hamiltonian H_I between system $\mathcal{S}$ and bath $\mathcal{B}$ [see (26) in *remark 3*].

Stress has been put on the completely positive condition of $K[\bullet]$. Then we have used that a Kossakowki-Lindblad *form* will be completely positive if this *form* is invariant under Davies's average procedure (30) [see Sect. 4]. Thus in the weak coupling approximation we have presented an explicit condition (37), in terms of an arbitrary H_I, in such a way that after the application of Davies's device the dynamics of the reduced system be the same as before applying Davies's device. We have exemplified this condition for the particular case of a spin system in contact with a bath [see (41)].

The second part of our paper is concerned with the Schrödinger-Langevin picture and its connection with Kossakowki-Lindblad generators for the reduced density matrix. From this point of view a breakthrough has been presented giving rise to a non-Markovian (linear) evolution equation for the *stochastic state vector* $|\Psi\rangle$ [and also for the equivalent *stochastic matrix* $\rho_{st}(t) \equiv |\Psi\rangle\langle\Psi|$]. We emphasize that in the present paper we were only concerned with a Markovian description. This stochastic picture has been studied for different models of the stochastic operator $\mathcal{F}(t)$ appearing in the Schrödinger-Langevin equation (42). In general $\mathcal{F}(t)$ is non-hermitian, so we have written this stochastic operator in terms of two hermitian operators $\mathcal{F}(t) = \tilde{H}(t) - i\tilde{U}(t)$. From this fact we have shown that the Schrödinger-Langevin dynamics has two contributions: *first* in addition to the reversible von Neumann term there is an extra random fluctuating contribution coming from $\tilde{H}(t)$ (which ultimately produces dissipation); *second* a purely irreversible contribution explicitly appears in terms of the sure linear operator U plus the stochastic operator $\tilde{U}(t)$ (which represents the fluctuations in the dissipation). A remarkable point is that in general both stochastic operators are correlated and this correlation depend on the specific model of interaction between the system and the bath. We emphasize that in the present approach the dissipation and the fluctuations are both assumed to be of the same order λ. Other characterizations concerning the dependence on the strength parameter λ can also be done in the context of the present picture.

From our stochastic non-Markovian operational equation (45) a perturbation theory in the Kubo number has been introduced to calculate the average—over the noise—of the stochastic matrix $\rho_{st}(t)$. In this context the linear operator U has been solved in a consistent way to assure trace conservation of the mean value of $\rho_{st}(t)$. This fact guarantees in mean value the normalization of the wave vector. Then in this way the reduced density matrix $\rho = \langle\rho_{st}(t)\rangle$ fulfills an evolution equation which has a Kossakowki-Lindblad *form* (Sect. 5.1). From this fact we have been able to interpret the dissipative operator D and the fluctuating superoperator $F[\bullet]$, appearing in the Kossakowki-Lindblad semigroup, as a function of $\tilde{H}(t)$ and $\tilde{U}(t)$ [see appendix B]. Also we have emphasized the parallelism between the Schrödinger-Langevin picture and the quantum semigroup. This follows, from appendix A, realizing that the structure of commutators and anti-commutator appearing in a Kossakowki-Lindblad generator appears also—in a natural way—from the Schrödinger-Langevin dynamics.

Later on at the end of our paper (Sects. 5.2 to 5.4), by putting $\mathcal{F}(t) = \sum_{\alpha=1}^{n} l_\alpha(t) V_\alpha$ we have assumed that the quantum bath could be represented in a sort of "noisy" way. This special form of $\mathcal{F}(t)$ has the advantage to work-out with cumulants of complex noises rather than with generalized cumulant for stochastic matrices. In this case, when $\mathcal{F}(t) = \sum_{\alpha=1}^{n} l_\alpha(t) V_\alpha$, the algebraic structure is formally the same as in (25), but where $\chi_{\alpha\beta}(-\tau)$ has to be replaced by the noise correlation $\langle\langle l_\alpha^*(t)\, l_\beta(t-\tau)\rangle\rangle$. Therefore, for this model of $\mathcal{F}(t)$ the Schrödinger-Langevin picture can be seen as giving rise to three remarkable applications:

$i)$ *The first* one is to choose different noise correlations as a possible way to build up Kossakowki-Lindblad generators that represent, in an empirical way, different physical situations.

$ii)$ *The second* one comes from the fact that we can map the stochastic dynamics with the trace-out dynamics. This is, we have found the *underlying stochastic non-markovian evolution* that in the markovian approximation give the same result that the trace-out dynamics. We remark that when $\mathcal{F}(t)$ is non-hermitian only the dissipative part (at any temperature) can be mapped, the quantum shift cannot be obtained from the Schrödinger-Langevin picture, but it can always be trivially incorporated into the stochastic dynamics. In the case when $\mathcal{F}(t)$ is hermitian both the shift and the dissipation can be mapped with the trace-out technique, but only at infinite temperature.

$iii)$ *The third* one is to give a stochastic dynamic that corresponds to a given algebraic structure; this can be tackled from the set of Eqs. (89).

We emphasize that all these facts open the possibility to work-out numerically with a *stochastic state vector* rather than the density matrix. This clearly reduces the computational time in solving complex dissipative systems. Finally this non-Markovian stochastic picture is a starting point to work-out higher perturbations which could go beyond the weak coupling approximation.

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Appendix A: On the Kossakowski-Lindblad generator

Here we are going to see other forms of writing the infinitesimal dissipative K-L generator (see Sect. 1). First define the superoperator $(A\,\mathcal{K}\,B)[\bullet]$ acting on the reduced density matrix as

$$(A\,\mathcal{K}\,B)[\rho] \equiv \frac{1}{2}\left([A\rho, B^\dagger] + [A, \rho B^\dagger]\right) \tag{A1}$$

With this notation the dissipative part of the K-L generator can be written as:

$$L_D[\rho] = \sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma}\,(V_\alpha\,\mathcal{K}\,V_\gamma)[\rho]\,. \tag{A2}$$

Thus if the basis is hermitian, *i.e.*, if $A = A^\dagger$ and $B = B^\dagger$ hold, the following relations can be written

$$\begin{aligned}
(A\,\mathcal{K}\,B)[\rho] + (B\,\mathcal{K}\,A)[\rho] &= \\
&-\frac{1}{2}\left([A,[B,\rho]] + [B,[A,\rho]]\right),\\
(A\,\mathcal{K}\,B)[\rho] - (B\,\mathcal{K}\,A)[\rho] &= \\
&\frac{1}{2}\left([A,\{B,\rho\}_+] - [B,\{A,\rho\}_+]\right).
\end{aligned} \tag{A3}$$

Using these formulas and the fact that matrix $a_{\alpha\gamma}$ is hermitian, we can put $a_{\alpha\gamma} \equiv b_{\alpha\gamma} + i\,c_{\alpha\gamma}$ where $b_{\alpha\gamma}$ is a symmetric matrix and $c_{\alpha\gamma}$ antisymmetric. Thus it is possible to write

$$\begin{aligned}
L_D[\rho] = &-\frac{1}{2}\sum_{\alpha,\gamma=1}^{N^2-1} b_{\alpha\gamma}\,[V_\alpha,[V_\gamma,\rho]]\\
&+\frac{i}{2}\sum_{\alpha,\gamma=1}^{N^2-1} c_{\alpha\gamma}\left[V_\alpha,\{V_\gamma,\rho\}_+\right].
\end{aligned} \tag{A4}$$

Therefore (if the basis V_α is hermitian) this expression is equivalent to the dissipative K-L generator if the matrices $b_{\alpha\gamma}$ and $c_{\alpha\gamma}$ are symmetric and antisymmetric respectively.

On the other hand, note that if we use the relations

$$\begin{aligned}
2AB &= \{A,B\}_+ + [A,B]\,,\\
2\,(A\rho B + B\rho A) &= \{A,\{B,\rho\}_+\}_+ - [A,[B,\rho]]\,,\\
2\,(A\rho B - B\rho A) &= [A,\{B,\rho\}_+] - \{A,[B,\rho]\}_+\,,
\end{aligned} \tag{A5}$$

which are valid for any operators A and B, it is possible to rewrite the operator D and the superoperator $F[\bullet]$ in the form

$$D = \frac{1}{4}\sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma}\left(\{V_\gamma^\dagger, V_\alpha\}_+ + [V_\gamma^\dagger, V_\alpha]\right),$$

$$\begin{aligned}
F[\rho] = \frac{1}{4}\sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma}\Big(&\left\{V_\alpha\{V_\gamma^\dagger,\rho\}_+\right\}_+ - [V_\alpha,[V_\gamma^\dagger,\rho]]\\
&+\left[V_\alpha,\{V_\gamma^\dagger,\rho\}_+\right] - \{V_\alpha,[V_\gamma^\dagger,\rho]\}_+\Big).
\end{aligned} \tag{A6}$$

Now if the basis is hermitian $V_\gamma = V_\gamma^\dagger$ and using again that $a_{\alpha\gamma} \equiv b_{\alpha\gamma} + i\, c_{\alpha\gamma}$ we have

$$\begin{aligned} L_D[\rho] = -\frac{1}{4}\sum_{\alpha,\gamma=1}^{N^2-1} b_{\alpha\gamma}\Big(\big\{\{V_\alpha, V_\gamma\}_+, \rho\big\}_+ \\ + [V_\alpha,[V_\gamma,\rho]] - \big\{V_\alpha, \{V_\gamma,\rho\}_+\big\}_+\Big) \\ + \frac{i}{4}\sum_{\alpha,\gamma=1}^{N^2-1} c_{\alpha\gamma}\Big(\{[V_\alpha, V_\gamma],\rho\}_+ \\ + \big[V_\alpha,\{V_\gamma,\rho\}_+\big] - \{V_\alpha,[V_\gamma,\rho]\}_+\Big). \quad \text{(A7)} \end{aligned}$$

In this expression only the real part is present if $a_{\alpha\gamma}$ is diagonal. Thus the terms of the generator corresponding to the real part, must have the form of a K-L. To see this fact we use again (A5) and note that

$$\begin{aligned} L_D[\rho] = -\frac{1}{4}\sum_{\alpha,\gamma=1}^{N^2-1} b_{\alpha\gamma}\Big(\big\{\{V_\alpha, V_\gamma\}_+, \rho\big\}_+ \\ - 2\left(V_\alpha\rho V_\gamma + V_\gamma\rho V_\alpha\right)\Big) + \frac{i}{4}\sum_{\alpha,\gamma=1}^{N^2-1} c_{\alpha\gamma}\big(\{[V_\alpha,V_\gamma],\rho\}_+ \\ + 2\left(V_\alpha\rho V_\gamma - V_\gamma\rho V_\alpha\right)\big). \quad \text{(A8)} \end{aligned}$$

Then, in the real part it is possible to recognize terms with the form of D and $F[\rho]$.

Appendix B: H_{eff}, D and $F[\bullet]$ as a function of $\tilde{H}(t)$ and $\tilde{U}(t)$

In this appendix the cumulant notation $\langle\!\langle \cdots \rangle\!\rangle$ has been dropped-out from any expression to simplify their formulas. In order to find H_{eff}, D and $F[\bullet]$ as a function of $\tilde{H}(t)$ and $\tilde{U}(t)$, introduce

$$\mathcal{F}(t) = \tilde{H}(t) - i\tilde{U}(t) \quad \text{(B1)}$$

in their expresions. From equation (55) we get for the deterministic unknown operator U

$$\begin{aligned} U = \lambda\int_0^\infty d\tau\Big(\big\{\tilde{U}(t), \tilde{U}(t-\tau)\big\}_+ \\ + i\big[\tilde{U}(t), \tilde{H}(t-\tau)\big]\Big). \quad \text{(B2)} \end{aligned}$$

From (B1) and (57) it follows that the effective hamiltonian is

$$\begin{aligned} H_{\text{eff}} = H_S - i\frac{\lambda^2}{2}\int_0^\infty d\tau\Big([\tilde{H}(t), \tilde{H}(t-\tau)] - [\tilde{U}(t), \tilde{U}(t-\tau)] \\ - i\big(\{\tilde{H}(t), \tilde{U}(t-\tau)\}_+ + \{\tilde{U}(t), \tilde{H}(t-\tau)\}_+\big)\Big). \quad \text{(B3)} \end{aligned}$$

The dissipative operator D reads

$$\begin{aligned} D = \frac{\lambda^2}{2}\int_0^\infty d\tau\Big(\{\tilde{H}(t), \tilde{H}(t-\tau)\}_+ + \{\tilde{U}(t), \tilde{U}(t-\tau)\}_+ \\ - i\big([\tilde{H}(t), \tilde{U}(t-\tau)] - [\tilde{U}(t), \tilde{H}(t-\tau)]\big)\Big) \quad \text{(B4)} \end{aligned}$$

and the fluctuating superoperator $F[\bullet]$ results

$$\begin{aligned} F[\bullet] = \lambda^2\int_0^\infty d\tau\Big(\big(\tilde{H}(t)\bullet\tilde{H}(t-\tau) + \tilde{H}(t-\tau)\bullet\tilde{H}(t)\big) + \big(\tilde{U}(t)\bullet\tilde{U}(t-\tau) + \tilde{U}(t-\tau)\bullet\tilde{U}(t)\big) \\ + i\big(\tilde{H}(t)\bullet\tilde{U}(t-\tau) - \tilde{U}(t-\tau)\bullet\tilde{H}(t)\big) - i\big(\tilde{U}(t)\bullet\tilde{H}(t-\tau) - \tilde{H}(t-\tau)\bullet\tilde{U}(t)\big)\Big) \quad \text{(B5)} \end{aligned}$$

Finally using (A5) this expression can be rewritten in the form:

$$\begin{aligned} F[\bullet] = \frac{\lambda^2}{2}\int_0^\infty d\tau\Big(\Big\{\tilde{H}(t), \big\{\tilde{H}(t-\tau), \bullet\big\}_+\Big\}_+ - \Big[\tilde{H}(t), \big[\tilde{H}(t-\tau), \bullet\big]\Big] \\ + \Big\{\tilde{U}(t), \big\{\tilde{U}(t-\tau), \bullet\big\}_+\Big\}_+ - \Big[\tilde{U}(t), \big[\tilde{U}(t-\tau), \bullet\big]\Big] \\ + i\Big(\Big[\tilde{H}(t), \big\{\tilde{U}(t-\tau), \bullet\big\}_+\Big] - \Big\{\tilde{H}(t), \big[\tilde{U}(t-\tau), \bullet\big]\Big\}_+\Big) \\ - i\Big(\Big[\tilde{U}(t), \big\{\tilde{H}(t-\tau), \bullet\big\}_+\Big] - \Big\{\tilde{U}(t), \big[\tilde{H}(t-\tau), \bullet\big]\Big\}_+\Big)\Big) \quad \text{(B6)} \end{aligned}$$

Now it is interesting to compare expressions (B4), (B6) with the dissipative K-L generator given in formula (A7) or alternatively expressions (B4), (B5) with (A8). Then we realize that the imaginary part comes from the *cross-correlation* between $\tilde{H}(t)$ and $\tilde{U}(t)$, but the real part comes from the *self-correlations* of $\tilde{H}(t)$ and $\tilde{U}(t)$. On the other hand any semigroup has a combination of commutator and anticommutator objects. These combinations appear in a natural way (in a second-order perturbation theory) from the Schrödinger-Langevin picture.

Appendix C: The fourth-order cumulant approximation

Here we are going to work out the Schrödinger-Langevin picture up to fourth order in the coupling parameter λ; then we show that also up to $\mathcal{O}(\lambda^4\tau_c^3)$ a K-L *form* for the evolution of the reduced density matrix ρ is obtained. The $H_{\rm eff}$, the *dissipative* operator D and the *fluctuating* superoperator $F[\bullet]$ are obtained in the general case. Also for a particular choice of the random operator $\mathcal{F}(t)$ the expression of a hermitian $a_{\alpha\gamma}$ is proved. Thereby a systematic way of calculating higher order corrections to $a_{\alpha\gamma}$ can be made in the present framework. These corrections are of interest when lowing down the temperature of the bath.

The notation and the methods are the same as in Subsect. 5.1. Starting from the stochastic multiplicative operational equation (50), the cumulant expansion [23] allows us to find a closed Markovian evolution for the average $\langle u(t)\rangle$ in $\mathcal{O}(\lambda^n\tau_c^{n-1})$

$$\frac{d}{dt}\langle u(t)\rangle = \left(A_o + \sum_{n=1}^{\infty}\lambda^n K_n\right)\langle u(t)\rangle \qquad \text{(C1)}$$

K_n is the n-th order generator. In Subsect. 5.1 (51) gives the corresponding contribution to $\mathcal{O}(\lambda^2\tau_c)$ in terms of K_1 and K_2. Here we give the next term in the cumulant expansion $\mathcal{O}(\lambda^4\tau_c^3)$, finding in this way a closed evolution equation for $\rho = \langle u(t)\rangle$ under the constrain $\mathrm{Tr}\rho(t) = 1$. We show that this trace conservation condition, once again, leads automatically to a K-L *form*, after solving in a consistent way the unknown dissipative (sure) operator U. This expansion can be done to any order λ^n but the algebraic manipulation is tedious. Making the same identifications as in (51) and (52) we write the next contribution from (C1). We assume that odd correlations of the random operator $\mathcal{F}(t)$ are null. Demanding trace conservation for ρ the operator U must fulfill (up to order λ^3) the self-consistent equation

$$\begin{aligned}2U = \lambda\int_0^{\infty} d\tau\big(&\langle\!\langle\mathcal{F}^\dagger(t)\,\mathcal{F}(t-\tau)\rangle\!\rangle \\ &- \langle\!\langle\mathcal{F}(t)\,\mathcal{F}(t-\tau)\rangle\!\rangle + h.c.\big) \\ + \lambda^2\int_0^{\infty} d\tau_1\int_{\tau_1}^{\infty} d\tau_2\big(&\langle\!\langle\mathcal{F}^\dagger(t)\,[\mathcal{F}(t-\tau_2),U(-\tau_1)]\rangle\!\rangle \\ &- \langle\!\langle\mathcal{F}(t)\,[\mathcal{F}(t-\tau_2),U(-\tau_1)]\rangle\!\rangle + h.c.\big) \qquad \text{(C2)}\end{aligned}$$

where we have used Heisenberg's representation for $U(-\tau)$ and for the random operator $\mathcal{F}(t)$ the same notation as in Subsect. 5.1. Now from (C2) we have to solve the sure hermitian operator U order by order in λ. The solution can be found in an iterative way. Note that the anticonmutative contribution $\lambda\{U_1,\bullet\}_+$ in (54) is of $\mathcal{O}(\lambda^2\tau_c)$, where U_1 reads from equation (55); then from (C2) the next iterative correction will give a contribution of $\mathcal{O}(\lambda^4\tau_c^3)$. Introducing the solution of U up to order λ^3 back into the cumulant expansion for $\dot\rho$ a K-L *form* to $\mathcal{O}(\lambda^4\tau_c^3)$ is obtained. Then the effective Hamiltonian and the *fluctuating* superoperator are

$$\begin{aligned}H_{\rm eff} = H_S - \frac{i}{2}\Big(\lambda^2\int_0^{\infty} d\tau\big(&\langle\!\langle\mathcal{F}(t)\,\mathcal{F}(t-\tau)\rangle\!\rangle \\ &- \langle\!\langle\mathcal{F}^\dagger(t-\tau)\,\mathcal{F}^\dagger(t)\rangle\!\rangle\big) \\ + \lambda^4\int_0^{\infty} d\tau_1\int_{\tau_1}^{\infty} d\tau_2\big(&\langle\!\langle\mathcal{F}(t)\,[\mathcal{F}(t-\tau_2),U_1(-\tau_1)]\rangle\!\rangle \\ &- \langle\!\langle[U_1(-\tau_1),\mathcal{F}^\dagger(t-\tau_2)]\,\mathcal{F}^\dagger(t)\rangle\!\rangle\big)\Big) \qquad \text{(C3)}\end{aligned}$$

$$\begin{aligned}F[\bullet] = \lambda^2\int_0^{\infty} d\tau\big(&\langle\!\langle\mathcal{F}(t)\bullet\mathcal{F}^\dagger(t-\tau)\rangle\!\rangle \\ &+ \langle\!\langle\mathcal{F}(t-\tau)\bullet\mathcal{F}^\dagger(t)\rangle\!\rangle\big) \\ + \lambda^4\int_0^{\infty} d\tau_1\int_{\tau_1}^{\infty} d\tau_2\big(&\langle\!\langle\mathcal{F}(t)\,[U_1(-\tau_1),\mathcal{F}^\dagger(t-\tau_2)]\rangle\!\rangle \\ &+ \langle\!\langle[\mathcal{F}(t-\tau_2),U_1(-\tau_1)]\,\mathcal{F}^\dagger(t)\rangle\!\rangle\big). \qquad \text{(C4)}\end{aligned}$$

Taking into account that $F^*[\mathbf{1}] \equiv D$ the *dissipative* operator D follows.

In the case when the bath can be represented as a linear combination of stationary complex stochastic processes times operators in $\mathcal{H}_S$, so $\mathcal{F}(t) = \sum_{\alpha=1}^{n} l_\alpha(t)V_\alpha$, the algebraic structure to $\mathcal{O}(\lambda^4\tau_c^3)$ is

$$\begin{aligned}a_{\alpha\gamma} = \lambda^2\sum_\beta\int_0^{\infty} d\tau\big(&\langle\!\langle l_\alpha(t)\,l_\beta^*(t-\tau)\rangle\!\rangle C_{\beta\gamma}^*(-\tau) \\ &+ \langle\!\langle l_\gamma^*(t)\,l_\beta(t-\tau)\rangle\!\rangle C_{\beta\alpha}(-\tau)\big) \\ + \lambda^4\sum_\beta\int_0^{\infty} d\tau_1\int_{\tau_1}^{\infty} d\tau_2\big(&\langle\!\langle l_\alpha(t)\,l_\beta^*(t-\tau_2)\rangle\!\rangle S_{\beta\gamma}^*(-\tau_1,-\tau_2) \\ &+ \langle\!\langle l_\gamma^*(t)\,l_\beta(t-\tau_2)\rangle\!\rangle S_{\beta\alpha}(-\tau_1,-\tau_2)\big), \qquad \text{(C5)}\end{aligned}$$

where the coefficients are

$$C_{\beta\gamma}(-\tau) = \mathrm{Tr}\left(V_\gamma^\dagger V_\beta(-\tau)\right),$$

$$S_{\beta\gamma}(-\tau_1,-\tau_2) = \mathrm{Tr}\left(V_\gamma^\dagger\,[V_\beta(-\tau_2),U_1(-\tau_1)]\right)$$

Note that Eq. (C5) assures hermiticity. The remarkable point is that up to this order the equation for ρ also has the K-L *form*. From this equation it is also possible to see that to $\mathcal{O}(\lambda^4\tau_c^3)$ there is a necessary condition for the matrix $a_{\alpha\gamma}$ to be positive (in a similar way see *remark* 3). Up to this order, and because odd correlations are null, the generator only depends on the two point correlations $\langle\!\langle\mathcal{F}^\dagger(t)\ \mathcal{F}(t-\tau)\rangle\!\rangle$. For higher order corrections the occurrence of four-point correlations are expected.

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(a) A linear map $\Lambda : \mathcal{A} \longrightarrow \mathcal{B}$, $\mathcal{A}$ and $\mathcal{B}$, C^* algebras, is said to be *completely positive* if the tensor product map $\Lambda^{(n)} = \Lambda \otimes \mathbf{1}_n : \mathcal{A} \otimes \mathcal{M}(n) \longrightarrow \mathcal{B} \otimes \mathcal{M}(n)$, is positive for all positive integers n.

(b) The dual generator is defined by the following relation: $Tr\left(K\left[\rho(t)\right]A\right) = Tr\left(\rho K^*\left[A(t)\right]\right)$.

(c) Let $|\Phi_i\rangle$ be a complete basis, then $\mathrm{Tr}\rho(t) = \left\langle \sum_i \langle \Phi_i \mid \Psi\rangle\langle\Psi \mid \Phi_i\rangle\right\rangle_{\mathcal{F},\mathcal{F}^\dagger} = \left\langle \sum_i \langle \Psi \mid \Phi_i\rangle\langle\Phi_i \mid \Psi\rangle\right\rangle_{\mathcal{F},\mathcal{F}^\dagger} = \left\langle ||\Psi||^2\right\rangle_{\mathcal{F},\mathcal{F}^\dagger}$ therefore $\mathrm{Tr}\rho(t) = 1 \Longrightarrow \left\langle ||\Psi||^2\right\rangle_{\mathcal{F},\mathcal{F}^\dagger} = 1$.

(d) Note that if $\mathcal{F}(t)$ were hermitian there should be (for all α, β) a couple (α', β') such that $l_{\alpha'}(t) = l^*_\alpha(t)$ and $l_{\beta'}(t) = l^*_\beta(t)$ with $V_{\alpha'} = V^\dagger_\alpha$, $V_{\beta'} = V^\dagger_\beta$.

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