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1999 J. Phys. A: Math. Gen. 32 631

(http://iopscience.iop.org/0305-4470/32/4/007)

On the quantum dissipative generator: weak-coupling approximation and stochastic approach

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Received 18 June 1998, in final form 14 October 1998

Abstract. For a quantum open system the so-called Schrödinger–Langevin picture has been revisited. In a second-order perturbation it is shown that a *non-Markovian* evolution for the stochastic state vector leads to a dissipative generator which has a Kossakowski–Lindblad form. In this context it is possible to analyse the completely positive condition. The equivalence of this picture with the *trace-out* technique in the weak coupling approximation has been proved.

1. Introduction

Associated with a quantum open system, many stochastic wavefunctions (SWF) have been introduced in recent years [1]. The approaches split into two groups: quantum diffusion models [2] and quantum jump models [3–5]. With the aid of these models it is possible to simulate the behaviour of individual quantum systems in a variety of situations like homodyne and photon counting measurements. Alternatively SWF has also been used in the context of wavepacket reduction [6, 7]. A remarkable point is that in all these models, it is possible to associate a stochastic matrix, given by the outer product of the SWF, such that in mean value it follows the evolution of the density matrix of the open system. Due to the fact that, in general, the dynamics is assumed Markovian, this evolution is given by a Kossakowsky–Lindblad (KL) generator [8–10]. This Markovian property can be seen in the models, by the use of white fluctuations.

On the other hand, it is well known that a quantum open system generally follows a non-Markovian evolution [11, 12]. More specifically, if we are observing the dynamics of a system (in a reduced Hilbert space $\mathcal{H}_S$) that is part of a big closed system, the reduced dynamics is non-Markovian. A canonical example is a system $\mathcal{S}$ in contact with a thermal bath $\mathcal{B}$. Nevertheless, owing to the difficulty that arises in dealing with a non-Markovian evolution, the usual approach is to propose a Markovian dynamics that approximates the original one. In this situation the most well known is the *Born–Markov approximation* [13–15] (or weak coupling approximation). As with SWF, much effort has been devoted to giving an interpretation of the Born–Markov approximation in a manner that resembles a stochastic evolution. The proposed models are based on the introduction of stochastic operators (quantum Langevin equations) [16–18]. In this context, a natural question arises: is it possible to give an SWF (in

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0305-4470/99/040631+16$19.50

the $\mathcal{H}_S$ of an open system) that follows a *non-Markovian evolution*, such that in the Markovian approximation it gives, for the reduced density matrix, the Born–Markov evolution? The answer is yes, and this is one of the main tasks of this paper, summarized in what we call the *Schrödinger–Langevin picture* (SL). This model follows the line of linear quantum diffusion models [19]; nevertheless we start by postulating a non-white (coloured) stochastic dynamics.

The SL model was first introduced by van Kampen [20], where he was only concerned with obtaining the *standard* KL generator, without looking at the effective Hamiltonian (the shift) or at the temperature dependence of the generator. Later on, in order to look at temperature dependence, non-white noises were introduced into the approach [21, 22].

In this paper we are going to tackle the previously-mentioned question and, in addition, we are going to show an interesting relation between the SL picture and KL generators. This arises because, in the context of a perturbation theory in the Kubo number, a dissipative generator of the KL form appears. We will use the expression *KL form* when the matrix that characterizes the generator—*the algebraic structure* $a_{\alpha\gamma}$—could be negative. Due to this, the question of positivity of the obtained generator arises. Since from the SL picture it is possible to build up several KL generators from a family of correlation functions, this last question can be addressed. In the same context, we investigate the possibility of assigning a stochastic non-Markovian evolution to a given positive generator, and then obtain the same conditions that appear in the Born–Markov approximation, analysing its positivity.

The paper is organized as follows. In section 2 we review KL generators and the Born–Markov approximation, in order to make, *a posteriori*, a comparison with the SL picture. Therefore the quantum generator of the semigroup will be written in an alternative form in terms of the dissipative operator D and the fluctuating superoperator $F[\bullet]$. From this we show that a KL form is always obtained if we *trace out* the bath variables of a total system $\mathcal{S} + \mathcal{B}$. This fact enlightens some difficulties posed by van Kampen and Oppenheim [17] in arriving at a KL form tracing out the bath variables. In appendix A, to see the positivity of this KL form, we analyse for a particular case (using Davies' device [23–25]) a condition on the interaction Hamiltonian between $\mathcal{S}$ and $\mathcal{B}$. In section 3 we introduce the SL picture, and a clear interpretation of the non-Markovian evolution for the *stochastic state vector* in terms of random operators is given. In section 3.1 we introduce a second-order perturbation theory from which a KL form is obtained. In sections 3.2–3.4 we analyse several dynamics that come from the different elections for the random operator $\mathcal{F}(t)$ appearing in the SL equation, and at the same time we show the problems that arise in trying to prove the equivalence of each of these dynamics with a Born–Markov approximation (trace-out). In section 3.5 we match the generator obtained from the SL picture with an arbitrary KL generator; thus a closed interpretation is pointed out. Finally we give the conclusions and perspectives. In appendix B we emphasize the parallelism between the SL picture and the quantum semigroup.

2. Quantum dissipative semigroups and weak coupling approximation

In quantum mechanics the most general form of a Markovian evolution, for a reduced density matrix $\rho(t)$, that gives rise to irreversibility, is the so-called Kossakoswki–Lindblad generator [8–10]. This generator gives a Markovian map that guarantees von Neumann's conditions on $\rho(t)$, and also provides a completely positive map on the trace class operators $\mathcal{T}$. This last condition is much stronger than the usual positivity†.

In an arbitrary finite-dimensional Hilbert space $\mathcal{H}_S$ ($\dim \mathcal{H}_S = N$) this KL generator in

† 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.

the Schrödinger picture is ($\hbar = 1$)

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

where H_{eff} is an effective Hamiltonian acting on the system $\mathcal{S}$; V_α, ($\alpha = 0, 1, \ldots, N^2 - 1$) is a basis in the C^* algebra of the $N \times N$ complex matrices $\mathcal{M}(N)$, $V_0 = \mathbf{1}$, and the *algebraic structure* $a_{\alpha\gamma}$ is a Hermitian positive-definite matrix characterizing the dissipation and the fluctuations of the *open quantum system* $\mathcal{S}$.

Remark 1. *This generator can trivially be written in the form*

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -\mathrm{i}[H_{eff}, \rho(t)] - \{D, \rho(t)\}_+ + F[\rho(t)] \tag{2}$$

where $\{\cdot, \cdot\}_+$ *denotes the anticommutator and*

$$D = \tfrac{1}{2} \sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma} V_\gamma^\dagger V_\alpha \qquad F[\bullet] = \sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma} V_\alpha \bullet V_\gamma^\dagger$$

D *will be called the dissipative operator and* $F[\bullet]$ *the fluctuating superoperator.*

An interpretation of these operators will be shown in the following sections. This splitting is frequently used in the context of the quantum jump approach [3, 4].

How to construct the KL generator for a given open quantum system is a well known problem. In principle we wish to find the KL generator from the underlying Hamiltonian dynamics for the *total closed system* (system $\mathcal{S}$+ bath $\mathcal{B}$)

$$H_T = H_S + H_B + \lambda H_I \tag{3}$$

but this is often technically impossible and therefore one needs to introduce some approximations in order to arrive to the quantum master equation for the reduced density matrix. Considering the total Liouville equation up to $\mathcal{O}(\lambda^2)$, the *Born–Markov approximation* gives the 'quantum master equation' [10, 13–16, 20]

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\mathrm{i}[H_S, \rho(t)] - \lambda^2 \int_0^\infty \mathrm{d}\tau \; \mathrm{Tr}_B([H_I, [H_I(-\tau), \rho(t) \otimes \rho_B^e]]) \tag{4}$$

where $H_I(-\tau) \equiv \mathrm{e}^{-\mathrm{i}\tau(H_B+H_S)} H_I \mathrm{e}^{\mathrm{i}\tau(H_B+H_S)}$, and ρ_B^e is the equilibrium density matrix of the bath $\mathcal{B}$. The trace is taken over the bath variables, thereby reducing the evolution in the Hilbert space $\mathcal{H}_T = \mathcal{H}_S \otimes \mathcal{H}_B$ to an evolution in $\mathcal{H}_S$.

Remark 2. *Equation (4) can be written in a KL 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 into the integrand of formula (4). We then get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\mathrm{i}[H_S, \rho(t)] - \frac{\lambda^2}{2} \int_0^\infty \mathrm{d}\tau \; \mathrm{Tr}_B([[H_I, H_I(-\tau)], \rho(t) \otimes \rho_B^e] \\ +[H_I, [H_I(-\tau), \rho(t) \otimes \rho_B^e]] + [H_I(-\tau), [H_I, \rho(t) \otimes \rho_B^e]]).\end{aligned} \tag{5}$$

Now, using that

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

equation (5) reduces to

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -\mathrm{i}[H_{eff}, \rho(t)] - \{D, \rho(t)\}_+ + F[\rho(t)] \tag{6}$$

with

$$H_{eff} = H_S - \mathrm{i}\frac{\lambda^2}{2}\int_0^\infty \mathrm{d}\tau\ \mathrm{Tr}_B([H_I, H_I(-\tau)]\rho_B^e) \tag{7}$$

$$D = \frac{\lambda^2}{2}\int_0^\infty \mathrm{d}\tau\ \mathrm{Tr}_B(\{H_I, H_I(-\tau)\}_+\rho_B^e) \tag{8}$$

$$F[\rho(t)] = \lambda^2 \int_0^\infty \mathrm{d}\tau\ \mathrm{Tr}_B(H_I\rho(t)\otimes\rho_B^e H_I(-\tau) + H_I(-\tau)\rho(t)\otimes\rho_B^e H_I). \tag{9}$$

Therefore (4) has the KL form because these last equations have the structure of equation (2).

In order to obtain the algebraic structure $a_{\alpha\gamma}$, let us assume that the interaction Hamiltonian H_I has the general expression

$$H_I = \sum_{\beta=1}^{n} V_\beta \otimes B_\beta \qquad n \leqslant N^2 - 1 \tag{10}$$

where V_β belong to $\mathcal{H}_S$ and B_β are bath operators. Using explicitly the fact that H_I is Hermitian, (7)–(9) can be rewritten in a slightly different manner; this fact will be useful for our future algebra. Introducing the notation

$$\chi_{\alpha\beta}(-\tau) \equiv \mathrm{Tr}_B(\rho_B^e B_\alpha^\dagger B_\beta(-\tau)) \tag{11}$$

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

$$H_{eff} = H_S - \mathrm{i}\frac{\lambda^2}{2}\sum_{\alpha\beta}\int_0^\infty \mathrm{d}\tau\ (\chi_{\alpha\beta}(-\tau)V_\alpha^\dagger V_\beta(-\tau) - \chi_{\alpha\beta}^*(-\tau)V_\beta^\dagger(-\tau)V_\alpha) \tag{12}$$

$$D = \frac{\lambda^2}{2}\sum_{\alpha\beta}\int_0^\infty \mathrm{d}\tau\ (\chi_{\alpha\beta}(-\tau)V_\alpha^\dagger V_\beta(-\tau) + \chi_{\alpha\beta}^*(-\tau)V_\beta^\dagger(-\tau)V_\alpha) \tag{13}$$

$$F[\bullet] = \lambda^2\sum_{\alpha\beta}\int_0^\infty \mathrm{d}\tau\ (\chi_{\alpha\beta}(-\tau)V_\beta(-\tau)\bullet V_\alpha^\dagger + \chi_{\alpha\beta}^*(-\tau)V_\alpha\bullet V_\beta^\dagger(-\tau)). \tag{14}$$

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

$$V_\beta(-\tau) \equiv \mathrm{e}^{-\mathrm{i}\tau H_S}V_\beta\mathrm{e}^{+\mathrm{i}\tau H_S} = \sum_{\gamma=1}^{N^2-1} C_{\beta\gamma}(-\tau)V_\gamma \tag{15}$$

and using the fact that the indices in (12)–(14) are dumb, equation (6) can be put as in the previous form (1), where now

$$H_{eff} = H_S - \mathrm{i}\frac{\lambda^2}{2}\sum_{\alpha\beta\gamma}\int_0^\infty \mathrm{d}\tau\ (\chi_{\gamma\beta}(-\tau)C_{\beta\alpha}(-\tau) - \chi_{\alpha\beta}^*(-\tau)C_{\beta\gamma}^*(-\tau))V_\gamma^\dagger V_\alpha \tag{16}$$

and the *algebraic structure* is given by

$$a_{\alpha\gamma} = \lambda^2\sum_\beta\int_0^\infty \mathrm{d}\tau\ (\chi_{\gamma\beta}(-\tau)C_{\beta\alpha}(-\tau) + \chi_{\alpha\beta}^*(-\tau)C_{\beta\gamma}^*(-\tau)). \tag{17}$$

Armed with these definitions we can now analyse the algebraic structure $a_{\alpha\gamma}$. From equation (17) it is simple to see that matrix $a_{\alpha\gamma}$ is Hermitian. Nevertheless, as we mentioned before, a necessary and sufficient condition to guarantee the completely positive condition on the map is $[a_{\alpha\gamma}] \geqslant 0$. Note that if we deal with a situation where the algebraic structure is not positive definite, it is always possible to introduce a *mathematical device*—due to Davies [10,23–25]—which leads to a KL generator, (see appendix A).

Remark 3. *A necessary condition to assure that the algebraic structure will be positive can be seen in the following way. 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* $n \leqslant N^2 - 1$, *and that the half-Fourier transform of the correlations of the bath are not zero. Then the set* $\{V_\beta\}_{\beta=1}^{n}$ *ought to be closed under Heisenberg representation, i.e.*

$$V_\beta(-\tau) \equiv \mathrm{e}^{-\mathrm{i}\tau H_S} V_\beta \mathrm{e}^{+\mathrm{i}\tau H_S} = \sum_{\gamma=1}^{m} C_{\beta\gamma}(-\tau) V_\gamma \qquad \textit{with} \quad m \leqslant n \tag{18}$$

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

When $m > n$, Sylvester's criterion shows that this affirmation can easily be proved by writing the elements of the matrix (17). A simple example is the spin–boson system with an interaction Hamiltonian proportional to the Pauli matrix σ_x. In this case condition (18) is not fulfilled, giving in this case a non-positive matrix $a_{\alpha\gamma}$.

Remark 4. *Introducing the definition*

$$\Gamma_{\alpha\beta}(-\tau) \equiv \mathrm{Tr}_B(\rho_B^e B_\alpha B_\beta(-\tau)) \tag{19}$$

in (7), the effective Hamiltonian can also be written in the following way

$$H_{eff} = H_S - \mathrm{i}\frac{\lambda^2}{2} \sum_{\alpha\beta} \int_0^\infty \mathrm{d}\tau \, (\Gamma_{\alpha\beta}(-\tau) V_\alpha V_\beta(-\tau) - \Gamma^*_{\alpha\beta}(-\tau) V^\dagger_\beta(-\tau) V^\dagger_\alpha). \tag{20}$$

Using in this expression the matrix $C_{\beta\gamma}(-\tau)$ (see definition (15)) results in

$$H_{eff} = H_S - \mathrm{i}\frac{\lambda^2}{2} \sum_{\alpha\beta\gamma} \int_0^\infty \mathrm{d}\tau \, (\Gamma_{\alpha\beta}(-\tau) C_{\beta\gamma}(-\tau) V_\alpha V_\gamma - \Gamma^*_{\alpha\beta}(-\tau) C^*_{\beta\gamma}(-\tau) V^\dagger_\gamma V^\dagger_\alpha). \tag{21}$$

Note that it was possible to write expression (21) because the interaction Hamiltonian is, of course, Hermitian. Then the use of the *pseudo-correlation* $\Gamma_{\alpha\beta}(-\tau)$ is only a change of notation. These formulae will be seen to be useful when looked at in the SL context.

3. The Schrödinger–Langevin picture

In this section we present the analysis concerning the SL picture. The starting point of this formalism is to postulate a non-Markovian stochastic multiplicative equation for the state vector of the quantum open system $\mathcal{S}$. This equation is written in terms of an unknown Hermitian linear operator U representing the dissipation, and a random operator $\mathcal{F}(t)$ representing the effect of the fluctuations as a result of the interaction with the 'external world'. The SL equation reads

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = [-\mathrm{i}H_S - \lambda(U + \mathrm{i}\mathcal{F}(t))]|\Psi\rangle \tag{22}$$

where λ is the coupling parameter and we assume that $\langle\mathcal{F}(t)\rangle = 0$. We also assume that the dissipation and the fluctuations are both of the same order in λ. Other characterizations [10,18] concerning the dependence on the strength parameter λ, can also be made in the context of the present picture.

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

$$\rho(t) = \langle \rho_{st}(t) \rangle. \tag{23}$$

The probabilistic weight of each realization $\rho_{st}(t)$ is characterized by the probability of the corresponding realization of the matrix noises. From (22) the stochastic matrix $\rho_{st}(t)$ evolves with the following non-Markovian equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{st}(t) = -\mathrm{i}[H_S, \rho_{st}(t)] - \lambda\{U, \rho_{st}(t)\}_+ - \mathrm{i}\lambda(\mathcal{F}(t)\rho_{st}(t) - \rho_{st}(t)\mathcal{F}^{\dagger}(t)). \tag{24}$$

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 split it in the form

$$\mathcal{F}(t) = \tilde{H}(t) - \mathrm{i}\tilde{U}(t) \tag{25}$$

where $\tilde{H}(t)$ and $\tilde{U}(t)$ are stationary stochastic Hermitian operators with zero mean value. Introducing this notation in equation (22) the evolution of the *stochastic state vector* can be rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = -\mathrm{i}(H_S + \lambda\tilde{H}(t))|\Psi\rangle - \lambda(U + \tilde{U}(t))|\Psi\rangle. \tag{26}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{st}(t) = -\mathrm{i}[H_S + \lambda\tilde{H}(t), \rho_{st}(t)] - \lambda\{U + \tilde{U}(t), \rho_{st}(t)\}_+ \tag{27}$$

which is nothing more than (24) written in terms of Hermitian operators. Now its physical interpretation is clear. From (27) note that:

(i) The von Neumann term has a total Hamiltonian with a random fluctuating contribution $\lambda\tilde{H}(t)$.
(ii) The purely irreversible term (anticommutator) has two contributions: the first one is a sure operator U and the second is a random operator $\tilde{U}(t)$ representing its fluctuations.

The 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 between $\mathcal{S}$ and the external world. When the external action is a thermal bath, this correlation is temperature dependent.

In order to get a closed equation for the reduced density matrix $\langle\rho_{st}(t)\rangle$ of $\mathcal{S}$, we will introduce a second-order perturbation theory in the coupling parameter λ. Then the unknown operator U will be found in a consistent way demanding $\mathrm{Tr}\langle\rho_{st}(t)\rangle = 1$, so this linear (sure) operator U will be, characterized by the correlations of the stochastic operators $\mathcal{F}(t)$ and $\mathcal{F}^{\dagger}(t)$. In this way we also give a closed evolution for the SWF (22).

3.1. The second-order cumulant approximation

The general stochastic equation (24), with an arbitrary multiplicative noise, can be written in the compact form

$$\frac{\mathrm{d}}{\mathrm{d}t}u(t) = \{A_o + \lambda A_1(t)\}u(t) \tag{28}$$

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 [20] (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 time evolution of $u(t)$, the average $\langle u(t)\rangle$ satisfies the closed Markovian equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle u(t)\rangle = \left\{A_o + \lambda\langle A_1(t)\rangle + \lambda^2\int_0^\infty \mathrm{d}\tau\ \langle\langle A_1(t)\mathrm{e}^{\tau A_o}A_1(t-\tau)\rangle\rangle\mathrm{e}^{-\tau A_o}\right\}\langle u(t)\rangle. \tag{29}$$

Then we can identify

$$\begin{aligned}\langle\, u(t)\rangle &\equiv \langle\rho_{st}(t)\rangle = \rho(t)\\ A_o &\equiv -\mathrm{i}[H_s, \bullet]\\ A_1(t) &\equiv -\{U, \bullet\}_+ - \mathrm{i}(\mathcal{F}(t)\bullet - \bullet\,\mathcal{F}^\dagger(t)).\end{aligned} \tag{30}$$

Thus, after a little algebra, (29) can be rewritten in the form

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\mathrm{i}[H_S, \rho(t)] - \lambda\{U, \rho(t)\}_+ + \lambda^2\int_0^\infty (\langle\langle\mathcal{F}(t)\rho(t)\mathcal{F}^\dagger(t-\tau)\rangle\rangle\\ +\langle\langle\mathcal{F}(t-\tau)\rho(t)\mathcal{F}^\dagger(t)\rangle\rangle\\ -\langle\langle\mathcal{F}(t)\mathcal{F}(t-\tau)\rangle\rangle\rho(t) - \rho(t)\,\langle\langle\mathcal{F}^\dagger(t-\tau)\mathcal{F}^\dagger(t)\rangle\rangle)\,\mathrm{d}\tau\end{aligned} \tag{31}$$

where all time-dependent operators are given in Heisenberg's representation, i.e. $\mathcal{F}(\tau) \equiv \mathrm{e}^{\mathrm{i}\tau H_S}\mathcal{F}\mathrm{e}^{-\mathrm{i}\tau H_S}$. Demanding the condition Tr $\rho(t) = 1$, the linear operator U must fulfil

$$\begin{aligned}U = \frac{\lambda}{2}\int_0^\infty \mathrm{d}\tau\ (\langle\langle\mathcal{F}^\dagger(t)\mathcal{F}(t-\tau)\rangle\rangle + \langle\langle\mathcal{F}^\dagger(t-\tau)\mathcal{F}(t)\rangle\rangle\\ -\langle\langle\mathcal{F}(t)\mathcal{F}(t-\tau)\rangle\rangle - \langle\langle\mathcal{F}^\dagger(t-\tau)\mathcal{F}^\dagger(t)\rangle\rangle).\end{aligned} \tag{32}$$

In this way the conservation in mean value of the stochastic wavefunction norm is also guaranteed. Introducing the expression for U back into (31), the evolution of $\rho(t)$ can be written in the form

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -\mathrm{i}[H_{eff}, \rho(t)] - \{D, \rho(t)\}_+ + F[\rho(t)] \tag{33}$$

where the Hamiltonian *shift* is characterized by the effective Hamiltonian

$$H_{eff} = H_S - \mathrm{i}\frac{\lambda^2}{2}\int_0^\infty \mathrm{d}\tau\ (\langle\langle\mathcal{F}(t)\mathcal{F}(t-\tau)\rangle\rangle - \langle\langle\mathcal{F}^\dagger(t-\tau)\mathcal{F}^\dagger(t)\rangle\rangle). \tag{34}$$

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

$$D = \frac{\lambda^2}{2}\int_0^\infty \mathrm{d}\tau\ (\langle\langle\mathcal{F}^\dagger(t)\mathcal{F}(t-\tau)\rangle\rangle + \langle\langle\mathcal{F}^\dagger(t-\tau)\mathcal{F}(t)\rangle\rangle) \tag{35}$$

$$F[\bullet] = \lambda^2\int_0^\infty \mathrm{d}\tau\ (\langle\langle\mathcal{F}(t)\bullet\mathcal{F}^\dagger(t-\tau)\rangle\rangle + \langle\langle\mathcal{F}(t-\tau)\bullet\mathcal{F}^\dagger(t)\rangle\rangle). \tag{36}$$

These equations show that the SL picture leads to an evolution equation for $\rho(t)$ that has the form of a KL generator. 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.

At this point we can get profit from the SL picture by modelling different objects $\langle\langle\mathcal{F}^\dagger(t)\mathcal{F}(t-\tau)\rangle\rangle$. However, to proceed with the calculation, a full matrix cumulant theory would be required [26]. To avoid this, we assume that the influence of the environment can be represented in a 'noisy way'. Therefore we write the stochastic operator $\mathcal{F}(t)$ as linear combinations of complex-random numbers times operators in $\mathcal{H}_S$

$$\mathcal{F}(t) = \sum_{\alpha=1}^{n} l_\alpha(t)V_\alpha \qquad n \leqslant N^2 - 1. \tag{37}$$

The numbers $l_\alpha(t)$ are stationary complex stochastic processes with zero mean value and non-white correlations. This model is the simplest form of $\mathcal{F}(t)$ because, in this way, only a cumulant theory of stochastic process is needed. Introducing (37) into the formula (34) we obtain for H_{eff}

$$H_{eff} = H_S - \mathrm{i}\frac{\lambda^2}{2}\sum_{\alpha\beta\gamma}\int_0^\infty \mathrm{d}\tau\,(\langle\langle l_\alpha(t)\, l_\beta(t-\tau)\rangle\rangle C_{\beta\gamma}(-\tau)V_\alpha V_\gamma - \text{h.c.}) \tag{38}$$

and from (35) and (36) the algebraic structure reads

$$a_{\alpha\gamma} = \lambda^2\sum_\beta\int_0^\infty \mathrm{d}\tau\,(\langle\langle l_\gamma^*(t)l_\beta(t-\tau)\rangle\rangle C_{\beta\alpha}(-\tau) + \langle\langle l_\alpha(t)l_\beta^*(t-\tau)\rangle\rangle C_{\beta\gamma}^*(-\tau)) \tag{39}$$

where the matrix $C_{\beta\gamma}(-\tau)$ was defined in (15) and $\langle\langle\cdots\rangle\rangle$ are the stationary correlations of the noises.

At this stage (as soon as a basis on $\mathcal{H}_S$ is chosen) the correlations can be selected, in an empirical way, to represent different physical situations [26, 27] and at the same time to assure positivity. Note that the positivity only depends on the correlations $\langle\langle l_\alpha^*(t)l_\beta(t-\tau)\rangle\rangle$ because the pseudo-correlations $\langle\langle l_\alpha(t)l_\beta(t-\tau)\rangle\rangle$ only appear in the expression of H_{eff}. We remark that from (38), (39) and for any $\mathcal{F}(t)$ (Hermitian or not, see (37)), if the correlations of the noises are white, the shift will cancel out and the dissipative generator will give the *standard* KL semigroup. Therefore a shift can only be obtained if the underlying dynamics is non-Markovian.

Now we wonder if it is possible to find complex stochastic processes in such a way as to match numerically an arbitrary given *algebraic structure*. Before going to the most general case (see section 3.5) we first answer this question when $a_{\alpha\gamma}$ comes from the trace-out technique (see (17)). In this case the 'external world' is a thermal bath, so we are going to explore if its influences can be represented in a 'noisy way' (coloured noise), and not just in the usual operator form [16, 26].

We note that (38) and (39) are formally equal to the terms obtained from the trace-out technique (see (21) and (17)) if we make the identification

$$\begin{aligned}\chi_{\alpha\beta}(-\tau) &\leftrightarrow \langle\langle l_\alpha^*(t)l_\beta(t-\tau)\rangle\rangle\\ \Gamma_{\alpha\beta}(-\tau) &\leftrightarrow \langle\langle l_\alpha(t)l_\beta(t-\tau)\rangle\rangle.\end{aligned} \tag{40}$$

Remark 5. *In principle we could ask how to find a set of correlated noises that fulfil, in a consistent way, relation (40). This problem does not have a direct solution. Therefore we will now analyse all the possible dynamics that come from the different elections for $\mathcal{F}(t)$: the Hermitian, anti-Hermitian, and the non-Hermitian case.*

3.2. 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 SL picture (22), is Hermitian. Using (25) 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 (32) it is simple to see that $U = 0$. Therefore from (26) and (27) the dynamics results

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = -\mathrm{i}(H_S + \lambda\tilde{H}(t))|\Psi\rangle \tag{41}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{st}(t) = -\mathrm{i}[H_S + \lambda\tilde{H}(t), \rho_{st}(t)]. \tag{42}$$

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*, gives rise to a KL 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 equations (34)–(36) will read

(i) the effective Hamiltonian

$$H_{eff} = H_S - \mathrm{i}\frac{\lambda^2}{2}\int_0^\infty \mathrm{d}\tau \, \langle\langle[\tilde{H}(t), \tilde{H}(t-\tau)]\rangle\rangle \tag{43}$$

(ii) the operator D

$$D = \frac{\lambda^2}{2}\int_0^\infty \mathrm{d}\tau \, \langle\langle\{\tilde{H}(t), \tilde{H}(t-\tau)\}_+\rangle\rangle \tag{44}$$

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

$$F[\bullet] = \lambda^2 \int_0^\infty \mathrm{d}\tau \, (\langle\langle\tilde{H}(t) \bullet \tilde{H}(t-\tau)\rangle\rangle + \langle\langle\tilde{H}(t-\tau) \bullet \tilde{H}(t)\rangle\rangle). \tag{45}$$

Note that in this case the SL picture is formally equivalent to the trace-out technique just by replacing $H_I \to \tilde{H}(t) = \tilde{H}(t)^\dagger$ (see (7)–(9)) and changing Tr$[\bullet]$ by a second cumulant object. Because we are assuming that $\mathcal{F}(t) = \tilde{H}(t) = \sum_{\alpha=1}^{n} l_\alpha(t) V_\alpha$ $(n \leqslant N^2 - 1)$, it is possible to assign a one-to-one correspondence between each operator of the bath and a complex noise (see (10)) in the form:

$$B_\alpha \leftrightarrow l_\alpha \qquad B_\alpha^\dagger \leftrightarrow l_\alpha^*. \tag{46}$$

Now our task is to find the complex stochastic process $l_\alpha(t)$ in such a way to match the corresponding correlation functions that come from the operators of the bath B_α, see (40). Before doing this, we note that owing to Hermiticity of $\tilde{H}(t)$, the expression of H_{eff} in (38) can be rewritten *only* in terms of $\langle\langle l_\alpha^*(t) l_\beta(t-\tau)\rangle\rangle$, and the resulting expression is the one in (16) changing quantum correlations by noise correlations. Then in order to match both generators it would only be required that

$$\mathrm{Tr}_B(\rho_B^e B_\alpha^\dagger B_\beta(-\tau)) \stackrel{?}{=} \langle\langle l_\alpha^*(t) l_\beta(t-\tau)\rangle\rangle. \tag{47}$$

If this were the case we would have found an algebraic structure and the H_{eff} from the SL picture, which would be numerically equal to the $a_{\alpha\gamma}$ and shift obtained from the trace-out technique. In what follows we will show that this is not possible to do. To show this fact we use rule (46) in the following cases

$$\begin{aligned} \chi_{\alpha\beta}(-\tau) &\equiv \mathrm{Tr}_B(\rho_B^e B_\alpha^\dagger B_\beta(-\tau)) \longleftrightarrow \langle\langle l_\alpha^*(t) l_\beta(t-\tau)\rangle\rangle \\ \chi_{\alpha'\beta'}^*(-\tau) &\equiv \mathrm{Tr}_B(\rho_B^e B_\beta(-\tau) B_\alpha^\dagger) \longleftrightarrow \langle\langle l_\alpha^*(t) l_\beta(t-\tau)\rangle\rangle \end{aligned} \tag{48}$$

where we have used that $B_{\alpha'} = B_\alpha^\dagger$, $B_{\beta'} = B_\beta^\dagger$.

From the rhs of (48) this mapping would be consistent, from the quantum point of view, if and only if

$$\chi_{\alpha\beta}(-\tau) = \chi_{\alpha'\beta'}^*(-\tau) \tag{49}$$

which means that

$$\mathrm{Tr}_B(\rho_B^e B_\alpha^\dagger B_\beta(-\tau)) = \mathrm{Tr}_B(\rho_B^e B_\beta(-\tau) B_\alpha^\dagger). \tag{50}$$

But in general this condition is not true because bath operators do not commute. Therefore, due to the non-commutativity of bath operators, an inconsistency to calculate the correlation functions $\langle\langle l_\alpha^*(t) l_\beta(t-\tau)\rangle\rangle$ results from assignation (47). Only at infinite temperature (where $\rho_B^e \equiv \mathrm{e}^{-\beta H_B}/\mathrm{Tr}[\mathrm{e}^{-\beta H_B}]$ is the identity operator in $\mathcal{H}_B$) could condition (50) be satisfied.

Then, at infinite temperature, the random Hamiltonian approach, with $\tilde{H}(t) = \sum_{\alpha=1}^{n} l_\alpha(t)V_\alpha$ (whose generator is characterized by (43) to (45)), would give exactly the same result as the one obtained from tracing-out techniques (with $H_I = \sum_{\alpha=1}^{n} V_\alpha \otimes B_\alpha$). We emphasize that the same conclusion was found by Abragam (without splitting the KL) in the context of nuclear magnetism [27].

Finally we remark that owing to the Hermiticity of $\tilde{H}(t)$ it follows that if $l_\alpha(t)$ were complex numbers there would be an index α' such that $l_{\alpha'}(t)$ would be the complex conjugate 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 an operator V_α is Hermitian the noise $l_\alpha(t)$ ought to be real. These are very restrictive conditions on the noises. This is the main reason why we cannot find a consistent map for a Hermitian model of $\mathcal{F}(t)$. In the next sections we analyse the cases when $\mathcal{F}(t)$ are anti-Hermitian and non-Hermitian.

3.3. Case when $\mathcal{F}(t)$ is an anti-Hermitian random operator

In this section we assume that the random operator $\mathcal{F}(t)$ is anti-Hermitian. Using (25) it is trivial to see that $\mathcal{F}(t) = -\mathcal{F}^\dagger(t)$ is equivalent to $\mathcal{F}(t) = -\mathrm{i}\tilde{U}(t)$ and $\tilde{H}(t) = 0$. Therefore the evolution is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = -\mathrm{i}H_S|\Psi\rangle - \lambda(U + \tilde{U}(t))|\Psi\rangle \tag{51}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{st}(t) = -\mathrm{i}[H_S, \rho_{st}(t)] - \lambda\{U + \tilde{U}(t), \rho_{st}(t)\}_+. \tag{52}$$

It is simple to see that the generator obtained from (52) is the same one as in the Hermitian case by performing the following changes: replace $\tilde{H}(t)$ by $\tilde{U}(t)$ and change the sign of the shift contribution (see appendix B). In this case the norm of the SWF is only conserved in mean value.

If we assume that $\mathrm{i}\mathcal{F}(t) = \tilde{U}(t) = \sum_{\alpha=1}^{n} l_\alpha(t)V_\alpha$, ($n \leqslant N^2 - 1$), and we try to match with the trace-out technique, the same problems as in the Hermitian case are found. That is, a correlation map cannot be established consistently because of the assignation (46). The responsibility of this one-to-one correspondence (46), is now the Hermiticity of $\tilde{U}(t)$. As in the Hermitian case $\mathcal{F}(t)$, if the correlations of the noises were white, the shift cancel out and the dissipative generator would give the *standard* KL semigroup. In the next section we analyse the most general case of the SL picture.

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

Contrary to what happens by tracing-out and also in the case when $\mathcal{F}(t)$ is Hermitian (or anti-Hermitian as in the previous section), here in the 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 stochastic theory, i.e. the generator (33) cannot be expressed only in terms of $\langle\langle l_\alpha^*(t)l_\beta(t-\tau)\rangle\rangle$.

Note that in this case, and if in particular we assume white noises

$$\langle\langle l_\alpha^*(t)l_\beta(t-\tau)\rangle\rangle = \delta_{\alpha\beta}\,\delta(\tau) \qquad \langle\langle l_\alpha(t)\,l_\beta(t-\tau)\rangle\rangle = 0 \tag{53}$$

from (32) we get $U = \frac{1}{2}\sum_\alpha V_\alpha^\dagger V_\alpha$, ($\lambda = 1$), then re-obtaining van Kampen's approach [20].

Now we want to solve the problem of finding noises $l_\alpha(t)$ in such a way that $a_{\alpha\gamma}$ and H_{eff} are numerically equal to the terms coming from the tracing-out technique. Since in this case we do not impose any restriction on $l_\alpha(t)$ (unlike in previous sections 3.2 and 3.3) it allows us to get a consistent *correlation mapping*.

We start by analysing the dissipative part. Assume that we have found noises such that the following equality is true

$$\mathrm{Tr}_B(\rho_B^e B_\alpha^\dagger B_\beta(-\tau)) \stackrel{?}{=} \langle\langle l_\alpha^*(t) l_\beta(t-\tau)\rangle\rangle. \tag{54}$$

In order to see if there is some contradiction in the assignation rule (54) we now proceed to do the same steps that we made in previous sections. 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 (54) it follows:

$$\begin{aligned}\chi_{\alpha\beta}(-\tau) &\equiv \mathrm{Tr}_B(\rho_B^e B_\alpha^\dagger B_\beta(-\tau)) \longleftrightarrow \langle\langle l_\alpha^*(t) l_\beta(t-\tau)\rangle\rangle \\ \chi_{\alpha'\beta'}^*(-\tau) &\equiv \mathrm{Tr}_B(\rho_B^e B_\beta(-\tau) B_\alpha^\dagger) \longleftrightarrow \langle\langle l_{\alpha'}(t) l_{\beta'}^*(t-\tau)\rangle\rangle.\end{aligned} \tag{55}$$

But because† $l_{\alpha'}(t) \neq l_\alpha^*(t)$ and $l_{\beta'}(t) \neq l_\beta^*(t)$ there is no inconsistency in (55). Furthermore, 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 associated (54) for $\chi_{\beta\alpha}(-\tau)$ does not impose any new restriction to build $\langle\langle l_\alpha^*(t) l_\beta(t-\tau)\rangle\rangle$.

In this manner, we arrive to the same dissipative KL form that was obtained from the tracing-out technique and without any inconsistency in the assignation rule (54). This is because in the present case it is *not possible* to establish the one-to-one mapping between bath operators B_α and complex noises $l_\alpha(t)$, as in (46).

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 $l_\alpha(t)$. Equality (54) gives only two equations to determine these four real correlations. This gives us two (free) degrees of freedom in the choice of the complex noises.

Now we proceed to check if there is some contradiction to try to match with the non-dissipative part of the generator (6). This task can be tackled because we still have two degrees of freedom to try to establish the following equality

$$\mathrm{Tr}_B(\rho_B^e B_\alpha B_\beta(-\tau)) \stackrel{?}{=} \langle\langle l_\alpha(t) l_\beta(t-\tau)\rangle\rangle. \tag{56}$$

Even when this formula only introduces two new restrictions, these are *inconsistent* with the previous one (54). To prove this fact note that, because the interaction Hamiltonian H_I is Hermitian, there always exist an α' such that $B_{\alpha'} = B_\alpha^\dagger$, $V_{\alpha'} = V_\alpha^\dagger$. Then, from the quantum point of view it is true that

$$\begin{aligned}\Gamma_{\alpha'\beta}(-\tau) &= \chi_{\alpha\beta}(-\tau) = \mathrm{Tr}_B(\rho_B^e B_\alpha^\dagger B_\beta(-\tau)) \\ \Gamma_{\alpha\beta}(-\tau) &= \chi_{\alpha'\beta}(-\tau) = \mathrm{Tr}_B(\rho_B^e B_\alpha B_\beta(-\tau))\end{aligned} \tag{57}$$

and this must be true for all couples (α,α') appearing in H_I. Therefore from (57) it follows that the noise correlations should fulfil

$$\begin{aligned}\langle\langle l_{\alpha'}(t) l_\beta(t-\tau)\rangle\rangle &= \langle\langle l_\alpha^*(t) l_\beta(t-\tau)\rangle\rangle \\ \langle\langle l_\alpha(t) l_\beta(t-\tau)\rangle\rangle &= \langle\langle l_{\alpha'}^*(t) l_\beta(t-\tau)\rangle\rangle.\end{aligned} \tag{58}$$

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

$$l_{\alpha'}(t) = l_\alpha^*(t). \tag{59}$$

But if this is so, $\mathcal{F}(t)$ would be Hermitian and the Hermitian case only matches the dissipative part from the trace-out technique at infinite temperature (see section 3.2). This is not the case of interest in the present section. Therefore in order not to get any inconsistency from (56) we have to match, simultaneously, both the irreversible and reversible part of the generator

† 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 $V_{\alpha'} = V_\alpha^\dagger$, $V_{\beta'} = V_\beta^\dagger$.

(6). Therefore, 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 mapping* is

$$\begin{aligned} &\chi_{\alpha\beta}(-\tau) \equiv \mathrm{Tr}_B(\rho_B^e B_\alpha^\dagger B_\beta(-\tau)) = \langle\langle l_\alpha^*(t) l_\beta(t-\tau)\rangle\rangle \\ &\langle\langle l_\alpha(t) l_\beta(t-\tau)\rangle\rangle = 0. \end{aligned} \tag{60}$$

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

We emphasize that with this assignation rule and from (38), the shift coming from the SL picture is null, therefore $H_{eff} = H_S$. Nevertheless, a shift can always be trivially incorporated into the stochastic dynamics. Also from (32) and (35) follows the identity

$$\lambda U = D. \tag{61}$$

Then the SL picture, which is in correspondence with the Born–Markov approximation, is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = [-\mathrm{i}H_S - D - \mathrm{i}\lambda\mathcal{F}(t)]|\Psi\rangle \tag{62}$$

where $\mathcal{F}(t) = \sum_{\alpha=1}^{n} l_\alpha(t) V_\alpha$, and where the noises are consistently determined by the correlating map (60). From (62) we can see, in the second-order approximation, that $\lambda U = D$ is responsible for the dissipation, and $\mathcal{F}(t)$ produces the fluctuating term $F[\bullet]$ in the KL form obtained from trace-out technique.

3.5. *Mapping an arbitrary algebraic structure*

In the previous section we have given an SL evolution to an open quantum system (where all the effects of the bath were introduced through non-white noises), that in the Markovian approximation corresponds to the generator of trace-out technique. Now we will investigate the possibility of assigning an SL dynamics (22) to a given *arbitrary* positive generator. This means that the algebraic structure obtained from SL (39) will be equal to a given algebraic structure $a_{\alpha\gamma}$, (i.e. an $M \times M$ positive Hermitian matrix where $M = N^2 - 1$). Then (39) provides a set of $\frac{1}{2}M(M+1)$ equations for the unknown noise correlations

$$a_{\alpha\gamma} = \lambda^2 \sum_\beta \int_0^\infty \mathrm{d}\tau\, (\langle\langle l_\gamma^*(t) l_\beta(t-\tau)\rangle\rangle C_{\beta\alpha}(-\tau) + \langle\langle l_\alpha(t) l_\beta^*(t-\tau)\rangle\rangle C_{\beta\gamma}^*(-\tau)). \tag{63}$$

For the case of a system in contact with a thermal bath, we have solved this non-trivial problem just by making the correlation mapping that we presented in previous sections. Obviously this method does not work in the general case.

For the general situation, we can assume that we have found a basis where the given $a_{\alpha\gamma}$ is diagonal; in addition, the noises can be assumed to be statistically independent from each other. Then from (63) we arrive at a simpler set of equations for the unknown noise correlations:

$$a_{\alpha\alpha} = \lambda^2 \int_0^\infty \mathrm{d}\tau\ \mathrm{Re}[\langle\langle l_\alpha^*(t) l_\alpha(t-\tau)\rangle\rangle C_{\alpha\alpha}(-\tau)] \tag{64}$$

and for $\alpha \neq \gamma$

$$0 = \int_0^\infty \mathrm{d}\tau\, (\langle\langle l_\gamma^*(t) l_\gamma(t-\tau)\rangle\rangle C_{\gamma\alpha}(-\tau) + \langle\langle l_\alpha(t) l_\alpha^*(t-\tau)\rangle\rangle C_{\alpha\gamma}^*(-\tau)) \tag{65}$$

which are equations for the half-Fourier transform of the correlations.

Remark 6. *We see that these expressions are trivially satisfied when noises are white, then it is always possible to associate a white stochastic dynamics with a KL generator. On the other hand, analysing (65), we see that in order to assign a colour dynamics to a given positive generator, the set $\{V_\beta\}_{\beta=1}^n$ ought to be closed under Heisenberg representation.*

We are aware that the same condition was also obtained in remark 3, analysing the Born–Markov approximation. As we have remarked before, the Born–Markov approach is an approximation for the non-Markovian evolution of an open quantum system. From these facts we conclude that the problem of the positivity of a generator is closely related with the type of underlying dynamics from which it is obtained. That is: *white dynamics* always leads to a positive generator; on the contrary to obtain a positive generator from an *underlying non-Markovian dynamics* the closure condition ought to be fulfilled.

4. Conclusions

This paper is concerned with the SL model emphasizing its connection with KL generators and the Born–Markov approximation. This picture, unlike other formalisms, starts postulating a non-Markovian (linear) evolution for the stochastic state vector $|\Psi\rangle$ of an open quantum system.

Introducing in the SL dynamics a perturbation theory in the Kubo number, we proved that the density matrix $\rho = \langle\rho_{st}(t)\rangle$ fulfils an evolution equation which has a KL form (section 3.1). At this point we made a fundamental assumption, that the environment causing fluctuations can be modelled by complex non-white noises, and we discarded the use of stochastic operator. In this case, when $\mathcal{F}(t) = \sum_{\alpha=1}^n l_\alpha(t)V_\alpha$, the SL picture gives rise to three remarkable points:

(i) First, it gives a stochastic non-Markovian evolution, as a possible way to build up KL generators that represent, in an empirical way, different physical situations and in addition assure positivity. Three different models of evolution are available: the Hermitian, anti-Hermitian and the full non-Hermitian case (sections 3.2–3.4).

(ii) The second point comes from the fact that it is possible to map the stochastic wave evolution 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 Born–Markov approximation—at any temperature—and where all the information of the quantum bath is introduced through correlated noises. Even more, we have been able to interpret, in the weak coupling approximation, the origin of the dissipative operator D and the fluctuating superoperator $F[\bullet]$.

(iii) Thirdly, it gives a stochastic wave evolution that in mean value corresponds to a given positive algebraic structure (section 3.5). In that section, we also proved that it is always possible to assign a white stochastic evolution to a given positive algebraic structure. On the other hand a coloured evolution can only be assigned if the set of operators $\{V_\beta\}$ satisfies closure under Heisenberg representation (this condition was also obtained in the trace-out, see remark 3).

Concerning the completely positive condition of the map, we have concluded, in section 3.5, that the positivity or not of the algebraic structure is closely related with the type of dynamics from which it is obtained. That is: *white* dynamics always leads to a positive generator; on the contrary, to obtain a positive generator from an *underlying non-Markovian dynamics* the closure condition ought to be fulfilled.

In appendix B we emphasized the parallelism between the SL picture and the quantum semigroup, highlighting that the structure of commutators and anticommutator appearing in a KL generator, also appears—in a natural way—from the SL picture.

In this paper we are only concerned with the Markovian approximation. Nevertheless, owing to the fact that our approach provides a non-Markovian SWF, this theory allows us to explore the consequences of having an underlying colour dynamics, and to see how this dynamics 'effectively' appears in the Markovian approach. As a matter of fact, the possibility to work out, *numerically*, with a non-white evolution for the stochastic state vector is under investigation. This type of evolution is useful in solid-state physics. On the other hand, how the different stochastic dynamics arise and how the correlations between $\tilde{H}(t)$ and $\tilde{U}(t)$ come out from different approximations (and physical situations) are interesting subjects which are under investigation. Finally, our non-Markovian stochastic picture is a plausible starting point to work out higher perturbations which could go beyond the weak coupling approximation.

Acknowledgments

MOC thanks grant CONICET PIP No 4948; AKC gives thanks for a Fellowship from CONICET; AAB would like to thank the Director of the Centro Atómico Bariloche for the kind hospitality received during the work carried out for this paper, the partial financial help from the Fundación Balseiro, and also gives thanks for a Fellowship from CONICOR.

Appendix A. Davies' device

If tracing out the bath variables does not lead to a quantum semigroup, it is always possible to introduce a *mathematical device*—due to Davies—which leads to a KL generator. This device is defined by

$$K^{\#} = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \exp(\mathrm{i}t[H_S, \bullet])K \exp(-\mathrm{i}t[H_S, \bullet]) \, \mathrm{d}t \tag{A1}$$

where K is the generator of the tracing-out technique in the weak coupling limit, and $\exp(\mathrm{i}t[H_S, \bullet])K \equiv \mathrm{e}^{\mathrm{i}tH_S} K \mathrm{e}^{-\mathrm{i}tH_S}$.

If the spectrum of H_S is non-degenerate, it is known that after Davies' 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 $F^{\#}[\bullet]$ and the lost term comes from $-\{D^{\#}, \bullet\}_+$.

In order to know which Hamiltonians $(S + B)$ could lead to positive KL generators, we are going to explore the *invariance* under Davies' device of the generators K. This invariance can be characterized in terms of the evolution of the interaction Hamiltonian $H_I(-\tau)$. A sufficient condition to guarantee the invariance of H_{eff}, D and $F[\bullet]$ is

$$\int_0^{\infty} \mathrm{d}\tau \ \mathrm{Tr}_B(H_I(-\tau)\rho \otimes \rho_B^e H_I) = \int_0^{\infty} \mathrm{d}\tau \ \mathrm{Tr}_B \left(\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \mathrm{d}t \ H_I(t-\tau)\rho \otimes \rho_B^e H_I(t) \right). \tag{A2}$$

Here we show condition (A2) in the particular case of a spin system $H_S = \alpha S_z B_z$ (S_z the z angular momentum and B_z a magnetic field), with an interaction Hamiltonian $H_I = \sum_{k=1}^{N-1} \sum_{q=-k}^{k} T_k^q \otimes B_k^q$, ($T_k^q$ are irreducible spherical tensor operators of rank k [15] acting on the system $\mathcal{S}$, and B_k^q are bath operators). Then the invariance is given by the condition

$$\int_0^{\infty} \mathrm{d}\tau \ \mathrm{Tr}_B(\rho_B^e B_k^q \cdot B_{k'}^{q'}(-\tau))\mathrm{e}^{-\mathrm{i}q'\tau} = 0 \qquad \text{for} \quad q' \neq -q. \tag{A3}$$

From (A3) we note that the effect of Davies' average is to eliminate the terms in K 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 is the invariance of the corresponding generators K guaranteed. Condition (A3) might be seen restrictive to few interaction Hamiltonians H_I, but we have found that this condition is a clear and plausible physical interpretation of what Davies' device produces in this model.

Appendix B. Quantum semigroup and SL picture

Here we are going to see another form of writing the infinitesimal dissipative KL generator, and we show how this form naturally arises in the SL picture. Note that if we use the relations

$$\begin{aligned}
&2AB = \{A, B\}_+ + [A, B] \\
&2(A\rho B + B\rho A) = \{A, \{B, \rho\}_+\}_+ - [A, [B, \rho]] \\
&2(A\rho B - B\rho A) = [A, \{B, \rho\}_+] - \{A, [B, \rho]\}_+
\end{aligned} \tag{B1}$$

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

$$\begin{aligned}
D &= \tfrac{1}{4} \sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma} (\{V_\gamma^\dagger, V_\alpha\}_+ + [V_\gamma^\dagger, V_\alpha]) \\
F[\rho] &= \tfrac{1}{4} \sum_{\alpha,\gamma=1}^{N^2-1} a_{\alpha\gamma} (\{V_\alpha \{V_\gamma^\dagger, \rho\}_+\}_+ - [V_\alpha, [V_\gamma^\dagger, \rho]] + [V_\alpha, \{V_\gamma^\dagger, \rho\}_+] - \{V_\alpha, [V_\gamma^\dagger, \rho]\}_+).
\end{aligned} \tag{B2}$$

Now if the basis is Hermitian, $V_\gamma = V_\gamma^\dagger$, and using the fact that matrix $a_{\alpha\gamma}$ is Hermitian, we can put $a_{\alpha\gamma} \equiv b_{\alpha\gamma} + \mathrm{i} c_{\alpha\gamma}$ where $b_{\alpha\gamma}$ is a symmetric matrix and $c_{\alpha\gamma}$ antisymmetric:

$$\begin{aligned}
L_D[\rho] = &-\tfrac{1}{4} \sum_{\alpha,\gamma=1}^{N^2-1} b_{\alpha\gamma} (\{\{V_\alpha, V_\gamma\}_+, \rho\}_+ + [V_\alpha, [V_\gamma, \rho]] - \{V_\alpha, \{V_\gamma, \rho\}_+\}_+) \\
&+ \frac{\mathrm{i}}{4} \sum_{\alpha,\gamma=1}^{N^2-1} c_{\alpha\gamma} (\{[V_\alpha, V_\gamma], \rho\}_+ + [V_\alpha, \{V_\gamma, \rho\}_+] - \{V_\alpha, [V_\gamma, \rho]\}_+)
\end{aligned} \tag{B3}$$

where $L_D[\bullet] = K[\bullet] + \mathrm{i}[H_{eff}, \bullet]$.

Now in the SL picture, we want find U, H_{eff}, D and $F[\bullet]$ as a function of $\tilde{H}(t)$ and $\tilde{U}(t)$. In order to do this, introduce (25) in the expressions (32) and (34)–(36). In what follows the cumulant notation $\langle\langle \cdots \rangle\rangle$ has been dropped for simplicity. From equation (32) for the deterministic unknown operator U we get

$$U = \lambda \int_0^\infty \mathrm{d}\tau \, (\{\tilde{U}(t), \tilde{U}(t-\tau)\}_+ + \mathrm{i}[\tilde{U}(t), \tilde{H}(t-\tau)]). \tag{B4}$$

From (34) it follows that the effective Hamiltonian is

$$\begin{aligned}
H_{eff} = H_S - \mathrm{i}\frac{\lambda^2}{2} \int_0^\infty \mathrm{d}\tau \, &([\tilde{H}(t), \tilde{H}(t-\tau)] - [\tilde{U}(t), \tilde{U}(t-\tau)] \\
&- \mathrm{i}(\{\tilde{H}(t), \tilde{U}(t-\tau)\}_+ + \{\tilde{U}(t), \tilde{H}(t-\tau)\}_+))
\end{aligned} \tag{B5}$$

and the dissipative operator D reads

$$\begin{aligned}
D = \frac{\lambda^2}{2} \int_0^\infty \mathrm{d}\tau \, &(\{\tilde{H}(t), \tilde{H}(t-\tau)\}_+ + \{\tilde{U}(t), \tilde{U}(t-\tau)\}_+ \\
&- \mathrm{i}([\tilde{H}(t), \tilde{U}(t-\tau)] - [\tilde{U}(t), \tilde{H}(t-\tau)])).
\end{aligned} \tag{B6}$$

Finally, with the aid of (B1) the fluctuating superoperator $F[\bullet]$ results:

$$\begin{aligned}F[\bullet] = \frac{\lambda^2}{2}\int_0^{\infty} \mathrm{d}\tau\, (&\{\tilde{H}(t), \{\tilde{H}(t-\tau), \bullet\}_+\}_+ - [\tilde{H}(t), [\tilde{H}(t-\tau), \bullet]] \\ &+\{\tilde{U}(t), \{\tilde{U}(t-\tau), \bullet\}_+\}_+ - [\tilde{U}(t), [\tilde{U}(t-\tau), \bullet]] \\ &+\mathrm{i}([\tilde{H}(t), \{\tilde{U}(t-\tau), \bullet\}_+] - \{\tilde{H}(t), [\tilde{U}(t-\tau), \bullet]\}_+) \\ &-\mathrm{i}([\tilde{U}(t), \{\tilde{H}(t-\tau), \bullet\}_+] - \{\tilde{U}(t), [\tilde{H}(t-\tau), \bullet]\}_+)).\end{aligned} \qquad \text{(B7)}$$

Now we compare expressions (B6), (B7) with the dissipative KL generator given in formula (B3). Then we see that any semigroup has a combination of commutator and anticommutator objects and these combinations appear in a natural way (in a second-order perturbation theory) from the SL picture. On the other hand we see 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 $\tilde{U}(t)$.

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