

Local generation of entanglement with Redfield dynamics

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Abstract

In phenomenological applications, time evolutions of Bloch-Redfield type are widely adopted for modelling open system dynamics, despite their non-positive preserving character: this physical inconsistency, that in general shows up at small times, is usually cured by suitably restricting the space of allowed initial states. Nevertheless, additional problems may arise in relation to entanglement: specifically, we show that Redfield dynamics can generate entanglement through a purely local action, and this unphysical effect can persist for finite times.

1 Introduction

Quantum systems immersed in large environments, typically heat baths, represent a paradigmatic framework for modelling quantum non-unitary dissipative dynamics in phenomenological applications. The time-evolution of such quantum systems can be obtained from the global system+environment dynamics by tracing over the environment (infinite) degrees of freedom and generally encodes decoherence and dissipation, including possible memory effects [1]-[11].

The derivation of such reduced time-evolution for the system alone from the microscopic system-environment interaction Hamiltonian is however notoriously tricky, leading to a plethora of different master equations, often generating physically inconsistent dynamics. In particular, even in the Markovian limit, obtained when the system-environment coupling is sufficiently weak and the environment correlations decay times are small with respect to the

characteristic time evolution of the system, the positivity of the system density matrix might not be in general preserved [12]-[15], with the remarkable exception of *quantum dynamical semigroups*, whose derivation is however based on a rigorous mathematical treatment [1]-[6].

Although acknowledged in the literature, these inconsistencies have been either dismissed as irrelevant for practical purposes or cured by adopting *ad hoc* prescriptions [16]-[24]. In- deed, time-evolutions of the so-called Bloch-Redfield type [12]-[15] are constantly used in applications, despite being non-positive [25]-[34].¹ As justification for this attitude, two facts are usually remarked: *i)* non-positivity is in general confined to small times, and *ii)* asymptotic thermalization is always guaranteed for such dynamics, while this is not always true for quantum dynamical semigroups, due to the constraints imposed by complete positivity, which however guarantees physical consistency in all situations.

In the following, we shall consider Markovian reduced dynamics of Redfield type in the case of a two-level system and point out further difficulties of such time-evolutions related to the presence of entanglement. More specifically, we shall study how the single qubit Redfield dynamics γ_t behaves when augmented to a factorized evolution $\Gamma_t = \text{id} \otimes \gamma_t$, describing the dynamics of the same qubit statistically coupled to a second ancillary qubit, which however remains completely inert in time, being subjected to the identity operation “id”. We find that the purely local, factorized evolution Γ_t can increase the entanglement of the two-qubit system, clearly an unphysical result.

Preliminary studies on these topics have been previously reported in [36]-[39], but limiting the considerations to small times and very specific models. Instead, general Redfield evolutions are here examined, explicitly showing that their inconsistencies in connection with entanglement generation are not a small-time effect, rather they remarkably persist for finite times. As a result, the use of Redfield type time-evolutions for modelling open system dynamics should be taken with great care.

2 Redfield dynamics

As previously remarked, we shall study the dynamics of a two-level system (qubit) immersed in an environment, modelled as a large heat bath in equilibrium at the inverse temperature β . Being (infinitely) large, the reservoir can be considered unaffected by the presence of the qubit and therefore in the reference Gibbs state:

$$\rho_B = \frac{e^{-\beta H_B}}{\text{Tr}_B[e^{-\beta H_B}]}, \quad (1)$$

where H_B is the Hamiltonian describing the bath dynamics.

On the other hand, in absence of the bath, the qubit dynamics is driven by a 2×2 Hamiltonian matrix H_S , that can be taken to assume the most general form:

$$H_S = \omega \mathbf{n} \cdot \boldsymbol{\sigma}, \quad (2)$$

¹This may lead to claim the existence of physical results that are instead the consequence of the non-positivity of the dynamics; see the discussion in [35], in relation to [33].

where σ_i , $i = 1, 2, 3$ are the Pauli matrices, n_i , $i = 1, 2, 3$ are the components of a three-dimensional unit vector, while 2ω represents the gap between the two qubit energy levels.

Within the standard open system paradigm [1]-[6], the interaction of the qubit with the bath is assumed to be weak and describable by a Hamiltonian H^I that is linear in both qubit and environment variables:

$$H^I = \sum_{i=1} \sigma_i \otimes B_i, \quad (3)$$

where B_i are suitable hermitian bath operators.

The total Hamiltonian H describing the complete system, the two-level system together with the heat bath, can thus be written as

$$H = H_S \otimes \mathbf{1}_B + \mathbf{1}_S \otimes H_B + \lambda H^I, \quad (4)$$

with λ a small coupling constant. It generates the time-evolution of the total density matrix ρ_{tot} , via the Liouville–von Neumann equation

$$\frac{\partial \rho_{\text{tot}}(t)}{\partial t} = -i[H, \rho_{\text{tot}}(t)], \quad (5)$$

starting at $t = 0$ from the initial configuration $\rho_{\text{tot}}(0) = \rho(0) \rho_B$, in absence of initial system-environment correlations.

Because of the weak coupling assumption, the dynamics of the reduced density matrix $\rho(t) = \text{Tr}_B[\rho_{\text{tot}}(t)]$ for the qubit is usually obtained through standard second-order approximations in the coupling λ and a *naive* Markovian limit. In this way, one finds that the qubit time-evolution is generated by a master equation of Bloch-Redfield type [12]-[15]:

$$\frac{\partial \rho(t)}{\partial t} = -i[H_S, \rho(t)] + D[\rho(t)], \quad (6)$$

with the dissipative part explicitly given by [5]:

$$D[\rho] = -\lambda^2 \int_0^\infty ds \text{Tr}_B [H^I(s), H^I, \rho \otimes \rho_B]. \quad (7)$$

where

$$H^I(s) = \sum_{i=1} \sigma_i(s) \otimes B_i(s), \quad (8)$$

with qubit and bath operators following their free evolution,

$$\sigma_i(s) = e^{iS_H s} \sigma_i e^{-iS_H s} = \sum_{j=1} U_{ij}(s) \sigma_j, \quad (9)$$

$$B_i(s) = e^{i s H_B} B_i e^{-i s H_B} , \quad (10)$$

and

$$U_{ij}(s) = n_i n_j + (\delta_{ij} - n_i n_j) \cos(2\omega s) - \varepsilon_{ijk} n_k \sin(2\omega s). \quad (11)$$

By introducing the bath two-point correlation functions,

$$G_{ij}(s) = \text{Tr}_B \rho_B B_i(s) B_j = G_{ji}(-s), \quad (12)$$

one can rewrite D in the more explicit form:

$$D[\rho] = -\lambda^2 \sum_{i,j} \int_0^\infty ds \left(G_{ij}(s) \sigma_i(s), \sigma_j \rho + G_{ji}(-s) \rho \sigma_j, \sigma_i(s) \right). \quad (13)$$

Using (9) and (11), this expression can be further brought to Kossakowski-Lindblad form:

$$D[\rho] = -i H_{LS} \rho + \sum_{i,j=1}^3 C_{ij} \sigma_j \rho \sigma_i - \frac{1}{2} \sigma_i \sigma_j \rho, \quad (14)$$

with

$$H_{LS} = \frac{\lambda^2}{2} \sum_{i,j=1}^3 \varepsilon_{ijk} C_{ij} - C_{ji}^* \sigma_k, \quad C_{ij} = \lambda^2 C_{ij} + C_{ji}^*, \quad (15)$$

and

$$C_{ij} = \sum_{k=1}^3 \int_0^\infty ds U_{ki}(s) G_{kj}(s). \quad (16)$$

The first contribution in (14) is of Hamiltonian form, the so-called *Lamb-shift*, that “renormalizes” the starting system Hamiltonian (2); instead, the second contribution is a purely dissipative one.

When written in this form, one realizes that the Redfield reduced time evolution γ_t generated by (6), (14) would be a physically consistent dynamics, provided the (hermitian) Kossakowski matrix \mathcal{C} is non-negative; indeed, in this case, γ_t would be a semigroup of completely positive maps. Unfortunately, because of the form (16) and the presence of the trigonometric functions in (11), in general C_{ij} possesses negative eigenvalues leading to finite dynamics γ_t that often are not even positive.

In order to explicitly expose such inconsistencies, it is convenient to choose the unit vector \mathbf{n} in (2) to point in the third direction, and assume that the heat bath is such that the correlation matrix (12) is diagonal, with only the elements G_{11} , G_{22} , G_{33} non-zero.² In this case, the Kossakowski matrix C_{ij} takes the form

$$C = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{21} & C_{22} & 0 \\ 0 & 0 & C_{33} \end{pmatrix}, \quad (17)$$

²This choice is not much restrictive and it will be further discussed in the next Section.

with

$$\begin{aligned}
C_{11} &= \frac{\lambda^2}{2} \int_{-\infty}^{\infty} ds e^{2i\omega s} [G_{11}(s) + G_{11}(-s)] , \\
C_{22} &= \frac{\lambda^2}{2} \int_{-\infty}^{\infty} ds e^{2i\omega s} [G_{22}(s) + G_{22}(-s)] , \\
C_{12} &= \lambda^2 \int_0^{\infty} ds \sin(2\omega s) [G_{12}^{22}(s) - G_{12}^{22}(-s)] = C_{21}^* , \\
C_{33} &= \lambda^2 \int_{-\infty}^{\infty} ds G_{33}(s) .
\end{aligned} \tag{18}$$

Similarly, the Lamb-shift contribution in (15) becomes proportional to σ_3 ,

$$H_{LS} = \frac{\lambda^2}{2} \delta\omega \sigma_3 , \quad \delta\omega = \int_0^{\infty} ds \sin(2\omega s) [G_{11}(s) + G_{11}(-s) + G_{22}(s) + G_{22}(-s)] , \tag{19}$$

so that, due to the presence of the heat bath, the initial qubit frequency ω gets a λ^2 -dependent shift:

$$\omega \rightarrow \tilde{\omega} = \omega + \frac{\lambda^2}{2} \delta\omega . \tag{20}$$

As we are dealing with a two-dimensional system, it proves convenient to adopt a vector-like representation by decomposing the qubit density matrix as

$$\rho = \frac{1}{2} \sigma_0 + \boldsymbol{\rho} \cdot \boldsymbol{\sigma} = \frac{1}{2} \begin{pmatrix} 1 + \rho_3 & \rho_1 - i\rho_2 \\ \rho_1 + i\rho_2 & 1 - \rho_3 \end{pmatrix} , \quad \text{Det}[\rho] = \frac{1}{4} \left(1 - \sum_{j=1}^3 \rho_j^2 \right) \geq 0 , \tag{21}$$

where σ_0 is the two-dimensional unit matrix, while $\boldsymbol{\rho}$ is the three-dimensional coherence or Bloch vector, of unit length for pure states. By representing ρ as a 4-vector $|\rho\rangle \equiv (1, \rho_1, \rho_2, \rho_3)$, the evolution equation (6), (14) can then be recast in a Schrödinger-like form

$$\partial_t |\rho(t)\rangle = -2L |\rho(t)\rangle , \tag{22}$$

where the 4×4 matrices L includes both the Hamiltonian and dissipative contributions:

$$L = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & a & b + \tilde{\omega} & 0 \\ 0 & b - \tilde{\omega} & \alpha & 0 \\ w & 0 & 0 & \gamma \end{pmatrix} , \tag{23}$$

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through $\tilde{\omega}$ in (20) and the real parameters:

$$\begin{aligned} a &= C_{22} + C_{33} , & b &= -\operatorname{Re} C_{12} , \\ \alpha &= C_{11} + C_{33} , & w &= -2 \operatorname{Im} C_{12} , \\ \gamma &= C_{11} + C_{22} . \end{aligned} \tag{24}$$

These parameters are not completely arbitrary. Since the environment state ρ_B is thermal, the correlations in (12) obey the so called *Kubo-Martin-Schwinger (KMS) condition* [40, 41]:

$$G_{ij}(t) = G_{ji}(-t - i\beta) , \quad (25)$$

that expresses the analyticity properties of thermal correlation functions with respect to time; it can be easily derived when H_B has discrete spectrum, but survive the thermodynamic limit and thus holds also for truly infinite environments. From it, and the explicit expressions (18), one then easily deduces the following relation:

$$\gamma - w = e^{-2\beta\omega} (\gamma + w) , \quad (26)$$

and thus, assuming γ nonvanishing,

$$\frac{w}{\gamma} = \frac{1 - e^{-2\beta\omega}}{1 + e^{-2\beta\omega}} . \quad (27)$$

In addition, as expressible in terms of positive combination of Fourier transform of two-point bath correlations, the parameters a , α and γ turn out to be nonnegative (*e.g.* see [1]).

In this particular case, the solution of (22) can be straightforwardly computed and the finite time evolution map $\gamma_t = e^{-2tL}$ explicitly obtained; starting from the initial values, ρ_1 , ρ_2 and ρ_3 , the components of the Bloch vector evolve in time according to:

$$\begin{aligned} \rho_1(t) &= M_{11}(t) \rho_1 + M_{12}(t) \rho_2 , \\ \rho_2(t) &= M_{21}(t) \rho_1 + M_{22}(t) \rho_2 , \\ \rho_3(t) &= e^{-2\gamma t} \rho_3 + \Lambda(t) , \end{aligned} \quad (28)$$

where

$$\begin{aligned} M_{11}(t) &= e^{-(a+\alpha)t} \cos \Omega t - \frac{a-\alpha}{\Omega} \sin \Omega t , \\ M_{22}(t) &= e^{-(a+\alpha)t} \cos \Omega t + \frac{a-\alpha}{\Omega} \sin \Omega t , \\ M_{12}(t) &= -2 e^{-(a+\alpha)t} \frac{b+\tilde{\omega}}{\Omega} \sin \Omega t , \\ M_{21}(t) &= -2 e^{-(a+\alpha)t} \frac{b-\tilde{\omega}}{\Omega} \sin \Omega t , \\ \Lambda(t) &= -\frac{w}{\gamma} (1 - e^{-2\gamma t}) , \end{aligned} \quad (29)$$

while

$$\Omega = \frac{4\tilde{\omega}^2 - 4b^2 - (a - \alpha)^2}{1/2},$$

(30)

is a positive frequency, as $\lambda = \omega$. From these explicit expressions, one immediately deduces that the Redfield dynamics asymptotically drives the system to the unique equilibrium state ρ_∞ , with Bloch vector components $\rho_\infty = (0, 0, -w/\gamma)$. Recalling (27), one immediately finds

$$\rho_\infty = \frac{e^{-\beta H_S}}{\text{Tr}[e^{-\beta H_S}]}, \quad (31)$$

so that the bath drives the qubit to an equilibrium Gibbs state at the bath temperature. As mentioned before, this characteristic of the Redfield dynamics makes it very appealing in applications.

On the other hand, the evolution (28) does not in general preserve the positivity of the qubit density matrix $\rho(t)$ for all times. Indeed, let us consider the derivative of $\text{Det}[\rho(t)]$ at the initial time $t = 0$:

$$\left. \frac{d}{dt} \text{Det}[\rho(t)] \right|_{t=0} = 2 \left(a \rho_1^2 + \alpha \rho_2^2 + 2b \rho_1 \rho_2 + \rho_3 \right) \left(w + \gamma \rho_3 \right). \quad (32)$$

For a pure initial state, such that $\rho_3 = 0$, $\rho_1^2 + \rho_2^2 = 1$ so that $\text{Det}[\rho] = 0$ (recall (21)), this derivative must be positive, otherwise negative probabilities would emerge as soon as the dynamics γ_t starts. However, the quadratic form $a \rho_1^2 + \alpha \rho_2^2 + 2b \rho_1 \rho_2$ in (32), with coefficients as in (24), need not be positive, so that indeed the dynamical map γ_t turns out to be in general non-positive.

It is interesting to notice that the origin of the lack of positivity-preservation of Redfield dynamics lies in the way the time-evolution generated by the free system Hamiltonian H_S interferes with the various approximations. Indeed, in absence of the free system evolution, $\omega = 0$, from (18) one immediately obtains $w = b = 0$. However, in this case the dynamical map γ_t turns out to be completely positive and not just simply positive.

As a cure to the appearance of negative probabilities, it has been proposed to restrict the space of initial conditions to those states ρ that remain positive under the action of the Redfield dynamics [16]-[19]. The general argument supporting this choice is that negative probabilities appear only at the start of the evolution, *i.e.* at short transient times, before the truly Markovian regime sets in, and therefore in a span of time not really covered by the Redfield approximation. However, as we shall see below, Redfield dynamics may be affected by additional, more serious inconsistencies in presence of entanglement when dealing with multipartite systems.

3 Redfield dynamics and entanglement

Let us now extend the treatment discussed in the previous section to a bipartite system, composed by two independent qubits, the first one just an inert ancilla, while the second one subjected to the action of a heat bath and evolving with the previously considered Redfield dynamics γ_t . The time evolution of the compound two-qubit system is then given

by $\Gamma_t = \text{id} \otimes \gamma_t$, where “id” represents the identity map. As initial two-qubit state, we shall choose an entangled state and follow its evolution under the dynamical map Γ_t .

Although this setting might at first sight appear artificial, the situation where a qubit, subjected to a noisy environment, is statistically correlated to another independent and dynamically inert ancilla is common in quantum information: it is the physical context where an entangled two-qubit state (*e.g.* a Bell state) is formed in the laboratory and, while one qubit is kept inert there, the second one is sent to another party via a noisy channel.

As the dynamics Γ_t acts locally on the two parties, no interaction between the two qubits is at work, a steady depletion of entanglement is expected. Instead, even starting from initial states whose positivity is preserved by Γ_t and whose reduced, one-qubit state remains positive under the Redfield dynamics γ_t , we shall see that the dynamical map Γ_t is able to periodically increase the two-qubit entanglement, even at finite times, clearly an unphysical behaviour.

In order to simplify the treatment, we shall limit our considerations to a special class of two-qubit density matrices, those with non-vanishing entries only along the two diagonals (in the two-qubit computational basis):

$$\rho = \begin{pmatrix} \rho_{11} & 0 & 0 & \rho_{14} \\ 0 & \rho_{22} & \rho_{23} & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 \\ \rho_{41} & 0 & 0 & \rho_{44} \end{pmatrix}, \quad (33)$$

with $\rho_{32} = \rho_{23}^*$ and $\rho_{41} = \rho_{14}^*$. Normalization requires $\rho_{11} + \rho_{22} + \rho_{33} + \rho_{44} = 1$, while positivity of ρ imposes:

$$\rho_{ii} \geq 0, \quad i = 1, 2, 3, 4, \quad \rho_{11}\rho_{44} - |\rho_{14}|^2 \geq 0, \quad \rho_{22}\rho_{33} - |\rho_{23}|^2 \geq 0. \quad (34)$$

Equivalently, a two-qubit density matrix can also be represented in the so-called *Fano form*, a generalization of the one-qubit decomposition in (21):

$$\rho = \frac{1}{4} \sigma_0 \otimes \sigma_0 + \sum_{i=1}^3 R_{0i} \sigma_0 \otimes \sigma_i + \sum_{i=1}^3 R_{i0} \sigma_i \otimes \sigma_0 + \sum_{i,j=1}^3 R_{ij} \sigma_i \otimes \sigma_j. \quad (35)$$

However, only elements from the set

$$X = \{ \sigma_0 \otimes \sigma_0, \sigma_0 \otimes \sigma_3, \sigma_3 \otimes \sigma_0, \sigma_1 \otimes \sigma_2, \sigma_2 \otimes \sigma_1, \sigma_1 \otimes \sigma_1, \sigma_2 \otimes \sigma_2, \sigma_3 \otimes \sigma_3 \}, \quad (36)$$

should have a nonvanishing contribution in order to reproduce the X-shape in (33), and one finds:

$$\begin{aligned}
R_{03} &= \rho_{11} - \rho_{22} + \rho_{33} - \rho_{44} , & R_{11} &= \rho_{14} + \rho_{41} + \rho_{32} + \rho_{23} , \\
R_{30} &= \rho_{11} + \rho_{22} - \rho_{33} - \rho_{44} , & R_{22} &= \rho_{32} + \rho_{23} - \rho_{14} - \rho_{41} , \\
R_{12} &= i \rho_{14} - \rho_{41} + \rho_{32} - \rho_{23} , & R_{33} &= \rho_{11} + \rho_{44} - \rho_{22} - \rho_{33} , \\
R_{21} &= i \rho_{14} - \rho_{41} - \rho_{32} + \rho_{23} .
\end{aligned} \tag{37}$$

Similarly, also the generator $\text{id} \otimes L$ of the two-qubit semigroup $\Gamma_t = \text{id} \otimes \gamma_t$ should have a specific form in order for Γ_t to preserve the same shape; this request puts some constraints on the generator L of the single-qubit dynamical map $\gamma_t = e^{tL}$. As discussed in the previous section, L can be in general decomposed into Hamiltonian and dissipative contributions:

$$L[\rho] = -i H, \rho + \sum_{i,j=1}^3 C_{ij} \sigma_i \rho \sigma_j - \frac{1}{2} \sum_{i,j=1}^3 \sigma_i \sigma_j, \rho , \tag{38}$$

for a generic hermitian 2-dimensional matrix H and 3×3 hermitian coefficient matrix C . However, only when H is proportional to σ_3 and C takes the form (17), the two-qubit density matrix will remain of the form (33) under the dynamical map $\text{id} \otimes e^{tL}$, thus justifying the choices made in the previous section.³ This result is the direct consequence of the specific decomposition of the Lie algebra $\text{su}(4)$, as generated by the 16 elements $\sigma_\mu \otimes \sigma_\nu$, $\mu, \nu = 0, 1, 2, 3$, induced by its subalgebra X ; indeed, $\text{su}(4) = X \oplus X^\perp$, where X^\perp is the complement set of X , together obeying the following algebraic relations under multiplication [42]:

$$X \cdot X \subset X , \quad X^\perp \cdot X^\perp \subset X , \quad X \cdot X^\perp \subset X^\perp , \quad X^\perp \cdot X \subset X^\perp . \tag{39}$$

Because of these relations, the set X is preserved by $\text{id} \otimes L$, and consequently by the finite dynamical map Γ_t it generates, only for the just specified choice of Hamiltonian and Kossakowski matrix.

An additional advantage of the X -shape density matrix in (17) is that its entanglement content can be explicitly evaluated through the computation of its concurrence $C[\rho]$ [43, 44]. Indeed, one finds:

$$C[\rho] = 2 \max \left\{ 0, |\rho_{23}| - \sqrt{\rho_{11}\rho_{44}}, |\rho_{14}| - \sqrt{\rho_{22}\rho_{33}} \right\} . \tag{40}$$

For sake of definiteness, in the following we shall assume to start at $t = 0$ with an entangled state for which $|\rho_{23}| > \sqrt{\rho_{11}\rho_{44}}$.

³To be precise, the form (17) of the Kossakowski matrix can be the result of a more general environment than the one considered in Section 2; specifically, one can allow generic two-point correlations for the B_1 and B_2 bath operators (with also $G_{12} = 0$), leaving only B_3 as an independent variable ($G_{13} = G_{23} = 0$). However, this slight generalization would not add new physical insights to the discussed results, while making the treatment more involved.

The evolution of the density matrix (33) under the dynamical map $\Gamma_t = \text{id} \otimes \gamma_t$, with γ_t as given by (28), (29), can be explicitly expressed as:

$$\begin{aligned}
\rho_{11}(t) &= \frac{1}{4} \left[1 + \Lambda(t) \left(1 + R_{30} \right) + e^{-2\gamma t} \left(R_{03} + R_{33} \right) \right], \\
\rho_{22}(t) &= \frac{1}{4} \left[1 - \Lambda(t) \left(1 + R_{30} \right) - e^{-2\gamma t} \left(R_{03} + R_{33} \right) \right], \\
\rho_{33}(t) &= \frac{1}{4} \left[1 + \Lambda(t) \left(1 - R_{30} \right) + e^{-2\gamma t} \left(R_{03} - R_{33} \right) \right], \\
\rho_{44}(t) &= \frac{1}{4} \left[1 - \Lambda(t) \left(1 - R_{30} \right) - e^{-2\gamma t} \left(R_{03} - R_{33} \right) \right], \\
\rho_{14}(t) &= \frac{1}{4} \left[M_{11}(t)R_{11} + M_{12}(t)R_{12} - M_{21}(t)R_{21} - M_{22}(t)R_{22} \right. \\
&\quad \left. - i \left[M_{21}(t)R_{11} + M_{22}(t)R_{12} + M_{11}(t)R_{21} + M_{12}(t)R_{22} \right] \right] = \rho_{41}^*(t), \\
\rho_{23}(t) &= \frac{1}{4} \left[M_{11}(t)R_{11} + M_{12}(t)R_{12} + M_{21}(t)R_{21} + M_{22}(t)R_{22} \right. \\
&\quad \left. + i \left[M_{21}(t)R_{11} + M_{22}(t)R_{12} - M_{11}(t)R_{21} - M_{12}(t)R_{22} \right] \right] = \rho_{32}^*(t).
\end{aligned} \tag{41}$$

First of all, one easily checks that the reduced density matrix for the second qubit obtained by tracing over the first one, $\rho^{(2)}(t) = \text{Tr}_1 \rho(t)$, remains positive for all times. Indeed, one finds:

$$\rho^{(2)}(t) = \frac{1}{2} \left[\sigma_0 + R_{03}(t)\sigma_3 \right], \quad R_{03}(t) = -\frac{W}{\gamma} \left[1 - e^{-2\gamma t} \right] + e^{-2\gamma t} R_{03}. \tag{42}$$

As $R_{03} \in [-1, 1]$, because of the positivity of the initial state, and, recalling (27), $0 \leq \gamma \leq 1$, one deduces that also $R_{03}(t) \in [-1, 1]$ for all times, thus assuring $\rho^{(2)}(t) \geq 0$, for any X-shaped initial state (33).

Instead, one expects that the positivity of a generic initial state (33) will not be preserved by the evolution map $\text{id} \otimes \gamma_t$ in (41), as the Redfield dynamics γ_t discussed in Section 2 is non-positive. In order to examine this issue in more detail, we shall focus on the following four-parameter family of initial two-qubit states:

$$\tilde{\rho} = \begin{pmatrix} \mu & 0 & 0 & u \\ 0 & v & iv & 0 \\ 0 & iv & 1 - 2\mu & v \\ 0 & 0 & v & 0 \end{pmatrix}, \tag{43}$$

$$u \geq 0, \quad v \geq 0, \quad 0 \leq 2\mu + v \leq 1, \quad u^2 \leq \mu^2, \quad v^2 \leq v(1 - 2\mu - v)$$

where μ, v, u and v are real constants satisfying the following inequalities, necessary for positivity:

$$\mu \geq 0, \quad v \geq 0, \quad 0 \leq 2\mu + v \leq 1, \quad u^2 \leq \mu^2, \quad v^2 \leq v(1 - 2\mu - v). \quad (44)$$

From (37), one further obtains: $R_{03} = -R_{30} = 1 - 2(\mu + \nu)$, $R_{12} = -R_{21} = 2\nu$, $R_{11} = -R_{22} = 2u$ and $R_{33} = 4\mu - 1$. As mentioned before, we shall also assume a non-vanishing concurrence, $C[\tilde{\rho}] = 2(|\nu| - \mu) > 0$.

By using the explicit time evolution given in (41), and taking for simplicity the bath temperature to be zero, so that, recalling (27), $w = \gamma$, one verifies by inspection that the diagonal elements of $\tilde{\rho}(t)$ remain non-negative for all times:

$$\begin{aligned}\tilde{\rho}_{11}(t) &= \mu e^{-2\gamma t}, & \tilde{\rho}_{33}(t) &= (1 - 2\mu - \nu) e^{-2\gamma t}, \\ \tilde{\rho}_{22}(t) &= \mu (1 - e^{-2\gamma t}) + \nu, & \tilde{\rho}_{44}(t) &= 1 - \mu - \nu - e^{-2\gamma t} (1 - 2\mu - \nu).\end{aligned}\quad (45)$$

Concerning the additional quadratic inequalities in (34), recall that the bath dissipative parameters a , b , α and γ in (24) are all proportional to λ^2 , which is assumed to be small. Consequently, one can neglect them with respect to the qubit frequency ω , and, as a result, take in practice $2\tilde{\omega}/\Omega \ll 1$. Within this approximation, from (41) one gets:

$$\begin{aligned}\tilde{\rho}_{11}(t)\tilde{\rho}_{44}(t) - |\tilde{\rho}_{14}(t)|^2 &= \mu e^{-2\gamma t} (1 - \mu - \nu - e^{-2\gamma t} (1 - 2\mu - \nu)) - u^2 e^{-2(a+\alpha)t} \\ &\geq \mu^2 e^{-2\gamma t} - u^2 e^{-2(a+\alpha)t} \geq 0,\end{aligned}\quad (46)$$

since $\mu^2 \geq u^2$, with the additional assumption $a + \alpha - \gamma \geq 0$. Similarly, one also finds:

$$\begin{aligned}\tilde{\rho}_{22}(t)\tilde{\rho}_{33}(t) - |\tilde{\rho}_{23}(t)|^2 &= (1 - 2\mu - \nu) e^{-2\gamma t} (\nu + \mu (1 - e^{-2\gamma t})) - v^2 e^{-2(a+\alpha)t} \\ &\geq \nu(1 - 2\mu - \nu) e^{-2\gamma t} - v^2 e^{-2(a+\alpha)t} \geq 0,\end{aligned}\quad (47)$$

since $\nu(1 - 2\mu - \nu) \geq v^2$. As a consequence, the four-parameter family of density matrices in (43) constitute a set of admissible initial states for the evolution $\text{id} \otimes \gamma_t$, with \otimes the non-positive Redfield dynamics (28), since they remain positive for all times.

Let now focus on the entanglement content of the evolving density matrix $\tilde{\rho}(t)$. We first consider the behaviour of the concurrence $C[\tilde{\rho}(t)]$ for small times. Using the explicit expressions in (41) expanded to first order in t , one finds:

$$C[\tilde{\rho}(t)] = \sqrt{\tilde{\rho}_{11}(t)\tilde{\rho}_{44}(t) - |\tilde{\rho}_{14}(t)|^2} = |\nu| - \mu + \gamma(3\mu + \nu - 1) - (a + \alpha)\nu + 2bu t + O(t^2). \quad (48)$$

It is sufficient to choose an initial state $\tilde{\rho}$ for which $1 - 2\mu - \nu \leq \mu$, and $u \leq -(a + \alpha)\nu/2b$ to immediately conclude that $C[\tilde{\rho}(t)]$ does increase in time as soon as the dynamics sets in, clearly an unphysical result for a Markovian dynamics.

A different situation occurs for non-Markovian single-qubit dynamics γ_t : in this case, by adding a second ancillary qubit, the resulting two-qubit time evolution, again of the factorized form $\text{id} \otimes \gamma_t$, might be able to increase the entanglement between the two qubits [45, 46]. As the “true”, unapproximated reduced qubit dynamics, obtained by just tracing over the bath degrees of freedom, is in general non-Markovian, one might then be tempted to conclude that the just signaled increase of entanglement of the Redfield dynamics actually reproduces

a real phenomenon. In fact, this is not the case, as the initial state of the three-party qubit+ancilla+bath total system, $\tilde{\rho} \otimes \rho_B$, is of the so-called “Markov type”, and for such states no non-Markovian reduced two-qubit dynamics exists able to augment at any latertime the entanglement of the initial two-qubit state [47].

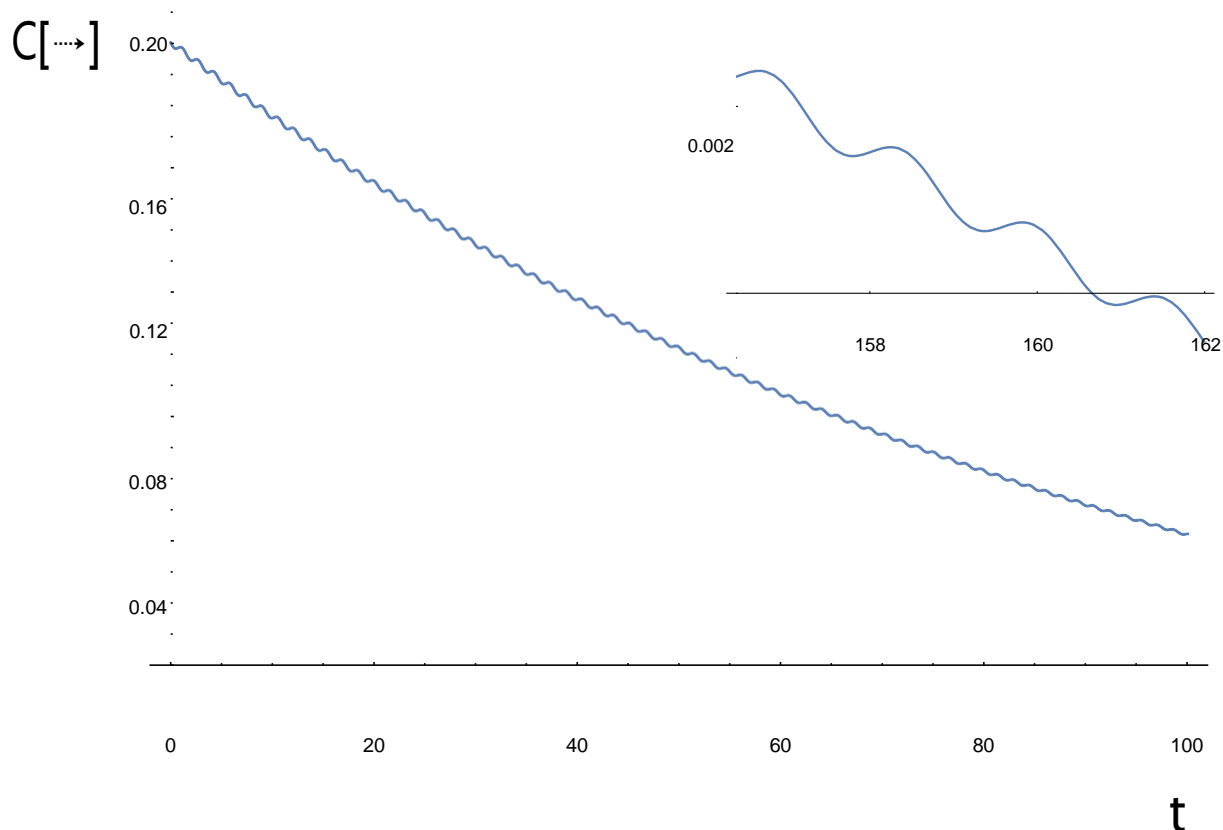


Figure 1: Behaviour of concurrence as a function of time in units $1/\omega$, with bath parameters $a/\omega = 0.005$, $b/\omega = 0.05$, $\alpha/\omega = 0.001$, $\gamma/\omega = 0.001$, $w/\gamma = 0.5$, for an initial state with $\mu = 0.025$, $\nu = 0.1$, $u = 0.02$ and $v = 0.125$; these values satisfy all the constraints (44) assuring the positivity of the initial density matrix, and the initial assumption of a weak coupled environment. The insert is an enlargement of the region where concurrence becomes zero: the oscillatory behaviour of concurrence is not a transient phenomenon, it persists for over 160 cycles.

The unphysical increase of entanglement signaled by (48) is a consequence of the non-positivity of the Redfield dynamics (see also the discussion in the next section) and as such is not limited to small times; indeed, Fig.1 displays the behaviour of the concurrence for an initial state belonging to the family in (43), in a range of constants μ , ν , u and v , different from that just examined in the small time regime, whose positivity is nevertheless preserved by the id γ_t dynamics. The bath is now at finite temperature, with bath parameters a , b , α , γ , w taken to be small with respect to ω , as $\lambda = \omega$ by assumption; time is measured in units of $1/\omega$. The plot shows an oscillatory shape, leading to a sudden death of entanglement, as expected

for a damping dynamics. However, at each cycle, concurrence increases, a

clear contradiction as the dynamical map is in factorized form. This periodic increase of entanglement is not a transient effect, disappearing after a few oscillations: it persists for very long times, as long as concurrence remains nonvanishing.

4 Discussion

In modelling the reduced dynamics of quantum systems weakly coupled to heat-baths, semi-groups of Bloch-Redfield type are often viewed as convenient choices. They are generated by master equations that can be readily obtained through second order approximations in the system-bath coupling and a naive Markovian limit.

However, for such dynamics, positivity of the system states is not guaranteed, as unphysical negative eigenvalues in the reduced density matrix begin to develop as soon as the dynamics starts. This “shortcoming” has not prevented the wide use of Redfield evolutions in applications, and various *ad hoc* prescriptions have been adopted in order to deal with the appearance of “negative probabilities”.

As the lack of positivity of the reduced density matrix occurs in general for small times, to avoid inconsistencies, one often used prescription is to restrict the possible system initial states to those for which the Redfield dynamics γ_t remains positive. Interestingly, this prescription works also when the system under study is statistically (but not dynamically!) coupled to another inert ancilla, provided the initial state is in separable form,

$\rho = \sum_i p_i \rho_i^{(1)} \otimes \rho_i^{(2)}$, $p_i \geq 0$, $\sum_i p_i = 1$, with $\rho_i^{(1)}$, $\rho_i^{(2)}$, admissible states for ancilla and system, respectively; indeed, in this case the time evolution is governed by the map $\text{id} \otimes \gamma_t$ and no negative eigenvalues can possibly develop.

Nevertheless, this prescription fails for entangled initial states, even when their positivity is preserved by the action of $\text{id} \otimes \gamma_t$, as further physical inconsistencies may arise. Indeed, as shown in the previous sections, in the case of a two-qubit system, the first inert, while the second evolving with a Redfield dynamics γ_t , their mutual entanglement can periodically increase under the action of $\text{id} \otimes \gamma_t$, a purely local operation. This unexpected phenomenon is not confined to the beginning of the dynamics: on the contrary, it persists for finite times, as long as the entanglement is not vanishing. The physical inconsistency of Redfield dynamics is therefore not limited to the initial occurrence of “negative probabilities”; rather, it manifests itself at finite times in the generation of entanglement through the action of local maps.

A similar phenomenon can be observed for the mutual information $I(S:A)$ of ancillary (A) + system (S) two-qubit model. This quantity provides the information about the total correlations present in the bipartite A + S system

$$I(S:A) = S(\rho_{SA} || \rho_S \otimes \rho_A), \quad (49)$$

where $S(\rho || \sigma) = \text{Tr}(\rho[\log \rho - \log \sigma])$ denotes a relative entropy, ρ_{SA} is an ancilla+system

state, while $\rho_A = \text{Tr}_S[\rho_{SA}]$ and $\rho_S = \text{Tr}_A[\rho_{SA}]$, the ancilla and system reduced density matrix. For a completely positive and trace perserving (CPTP) semigroup one obviously has

$$\frac{d}{dt} S \rho_{SA}(t) || \rho_S(t) \otimes \rho_A(t) \leq 0, \quad (50)$$

where $\rho_{SA}(t) = (e^{tL} \otimes \text{id})[\rho_{SA}]$, *i.e.* the total correlations present in the initial state ρ_{SA} monotonically decrease. Simple analysis shows that for the Redfield dynamics the inequality (50) is again violated. Moreover, it is violated even for times when the dynamics is already completely positive.

It is worth stressing that this unphysical behaviour also affects Redfield evolutions of more general form, of type $\gamma_t \otimes \gamma_t$. These dynamical maps describe the reduced dynamics of two equal, independent, non-interacting systems, both immersed in a common environment; as $\gamma_t \otimes \gamma_t = \text{id} \otimes \gamma_t \otimes \gamma_t \otimes \text{id}$, local generation of entanglement would also occur in this more general setting.⁴ In addition, through straightforward extensions of the bipartite setting, Redfield dynamics will clearly show similar inconsistencies also in the case of multipartite systems.

These considerations seems to suggest the presence of an intrinsic incompatibility of Red- field type dynamics with entangled states. As mentioned before, the origin of such inconsistency has to be found with the way the free evolution generated by the system Hamiltonian interferes with the approximations used to derive the Redfield dynamics. This is clearly indicated by the oscillating behaviour of concurrence in Fig.1, with a period $1/\omega$, the inverse of the free system energy unit. The same periodicity can be found in the time behaviour of the Choi matrix, $\text{id} \otimes \gamma_t [P_+]$, where $P_+ = |\psi_+\rangle \langle \psi_+|$, with $|\psi_+\rangle = (|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle) / \sqrt{2}$, $\sigma_3|i\rangle = (-1)^{i+1}|i\rangle$, $i = 0, 1$, whose positivity signals the complete positivity of the dynamical map γ_t . For the Redfield evolution discussed above, the Choi matrix starts having negative eigenvalues as soon as the dynamics starts, becoming positive only at longer times, after having oscillating between being negative and positive.

It should be stressed, however, that a Redfield semigroup $\gamma_t = e^{tL}$ even when becomes completely positive is still not CP-divisible, *i.e.* the intermediate map (a propagator) $\gamma_{t,s} = e^{(t-s)L}$ for $t > s$ need not be completely positive; actually, for small τ the map $e^{\tau L}$ violates even positivity. Hence, although the Redfield semigroup becomes CPTP after some finite time T , it still violates CP-divisibility and displays typical non-Markovian dynamical effects such as non-monotonicity of concurrence and mutual information. In a sense the dynamical map for $t > T$ remembers that initially the very condition of positivity was violated.

One way to deal with all these problems is through the precise mathematical treatment devised by Davies,⁵ that in the particular case discussed in the previous sections amounts to

⁴In this regard, it might be worth recalling that the dynamical map $\gamma_t \otimes \gamma_t$ is positive-preserving if and only if γ_t is completely positive [48].

⁵For a detailed derivation and discussion, *e.g.* see [1]-[6].

substitute the dissipative generator D in (6), (7), with the following ergodic average:

$$\tilde{D} = \lim_{T \rightarrow +\infty} \frac{1}{2T} \int_{-T}^{+T} dt e^{-\tau L_S} \circ D \circ e^{\tau L_S}, \quad (51)$$

where $L_S[\cdot] = -i H_S \cdot$ is the generator of the free Hamiltonian system dynamics. This average operation will then transform the 4×4 matrix generator L in (23) into a new one \tilde{L} , of the same form as (23), with $b = 0$ and a and α replaced by $(a + \alpha)/2$. As a , α , γ are positive, the family of transformations $\tilde{\gamma}_t$ generated by \tilde{L} form a semigroup of completely positive maps, having as asymptotic state the same Gibbs equilibrium state (31) of the original Redfield evolution. In this case, no inconsistencies will possibly arise as such dynamics are perfectly compatible with the presence of entanglement, in all possible physical situations, thus suggesting a safer alternative to the use of Redfield dynamics, at least within the domain of applicability of the Davies prescription [49].

References

- [1] R. Alicki, K. Lendi, *Quantum Dynamical Semi-Groups and Applications*, Lect. Notes Phys. **717**, (Springer-Verlag, Berlin, 2007)
- [2] E.B. Davies, *Quantum Theory of Open Systems*, (Academic Press, New York, 1976)
- [3] V. Gorini, A. Frigerio, M. Verri, A. Kossakowski and E.C.G. Surdarshan, Rep. Math. Phys. **13** (1978) 149
- [4] H. Spohn, Rev. Mod. Phys. **53** (1980) 569
- [5] F. Benatti and R. Floreanini, Int. J. Mod. Phys. B **19**, 3063 (2005)
- [6] A. Rivas and S.F. Huelga, *Open Quantum Systems* (Springer, Heidelberg, 2012)
- [7] W.H. Louisell, *Quantum Statistical Properties of Radiation*, (Wiley, New York, 1973)
- [8] C.W. Gardiner and P. Zoller, *Quantum Noise*, II ed., (Springer, Berlin, 2000)
- [9] M.O. Scully and M.S. Zubairy, *Quantum Optics* (Cambridge University Press, Cambridge, 1997)
- [10] R.R. Puri, *Mathematical Methods of Quantum Optics*, (Springer, Berlin, 2001)
- [11] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002)
- [12] F. Bloch, Phys. Rev. **105** (1957) 1206
- [13] A.G. Redfield, IBM J. Res. Dev. **1** (1957) 19

- [14] A.G. Redfield, *Adv. Magn. Reson.* **1** (1965) 1
- [15] C.P. Slichter, *Principle of Magnetic Resonance* (Springer-Verlag, Berlin, 1990)
- [16] S. Gnutzmann and F. Haake, *Z. Phys. B* **10** (1996) 263
- [17] A. Suarez, R. Silbey and I. Oppenheim, *J. Chem. Phys.* **97** (1992) 5101
- [18] P. Gaspard and M. Nagaoka, *J. Chem. Phys.* **111** (1999) 5668
- [19] J. Wielkie, *J. Chem. Phys.* **114** (2001) 7736
- [20] R.S. Whitney, *J. Phys. A* **41** (2008) 175304
- [21] D. Farina and V. Giovannetti, *Phys. Rev. A* **100** (2019) 012107
- [22] D. Davidovic, *Quantum* **4** (2020) 326
- [23] A. S. Trushechkin, *Proc. Steklov Inst. Math.* **313** (2021) 246
- [24] T. Becker, L.-N. Wu and A. Eckardt, *Phys. Rev. E* **104** (2021) 014110
- [25] W.T. Pollard, A.K. Felts and R.A.Friesner, *Adv. in Chem. Phys.*, **93** (1996) 77
- [26] M. Yang and G.R. Fleming, *Chem. Phys.* **282** (2002) 163
- [27] A. Ishizaki and G.R. Fleming, *J. Chem. Phys.* **130** (2009) 234110
- [28] J. Jeske and J.H. Cole, *Phys. Rev. A* **87** (2013) 052138
- [29] J. Thingna, J.-S. Wang and P. Hänggi, *Phys. Rev. E* **88** (2013) 052127
- [30] J. Jeske, D.J. Ing, M.B. Plenio, S.F. Huelga and J.H. Cole, *J. Chem. Phys.* **142** (2015) 064104
- [31] A. Purkayastha, A. Dhar and M. Kulkarni, *Phys. Rev. A* **93** (2016) 062114
- [32] A. Dodin, T. Tscherbul, R. Alicki, Amar. and P. Brumer, *Phys. Rev. A* **97** (2018) 013421
- [33] G. Guarnieri, M. Kolár and R. Filip, *Phys. Rev. Lett.* **121** (2018) 070401
- [34] R.Hartmann and W.T. Strunz, *Phys. Rev. A* **101** (2020) 012103
- [35] M. Cattaneo and G. Manzano, Comment on "Steady-State Coherences by Composite System-Bath Interactions", arXiv:2106.09138
- [36] F. Benatti, R. Floreanini and M. Piani, *Phys. Rev. A* **67** (2003) 042110
- [37] F. Benatti, R. Floreanini and S. Breteaux, *Laser Phys.* **16** (2006) 1395

- [38] S. Anderloni, F. Benatti and R. Floreanini, *J. Phys. A* **40** (2007) 1625
- [39] F. Benatti and R. Floreanini, *Int. J. Quantum Inf.* **5** (2007) 189
- [40] W. Thirring, *Quantum Mathematical Physics: Atoms, Molecules and Large Systems*, (Springer-Verlag, Berlin, 2002)
- [41] O. Bratteli and D.W. Robinson, *Operator Algebras and Quantum Statistical Mechanics* (Springer, Berlin, 2002)
- [42] N. Quesada, A. Al-Quasimi and D.F.V. James, *J. Mod. Opt.* **59** (2012) 1322
- [43] C.H. Bennett, D.P. DiVincenzo, J.A. Smolin and W.K. Wootters, *Phys. Rev. A* **54** (1996) 3824
- [44] W.K. Wootters, *Phys. Rev. Lett.* **80** (1998) 2245
- [45] R. Lo Franco, B. Bellomo, S. Maniscalco and G. Compagno, *Int. J. Mod. Phys. B* **27** (2013) 1345053
- [46] L. Aolita, F. de Melo and L. Davidovich, *Rep. Prog. Phys.* **78** (2015) 042001
- [47] I. Sargolzahi, *Quantum Inf. Process* **17** (2018) 138
- [48] F. Benatti, R. Floreanini and R. Romano, *J. Phys. A* **35** (2002) L551
- [49] M. Merkli, *Ann. of Phys.* **412** (2020) 167996