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Implications of non-Markovian quantum dynamics for the Landauer bound

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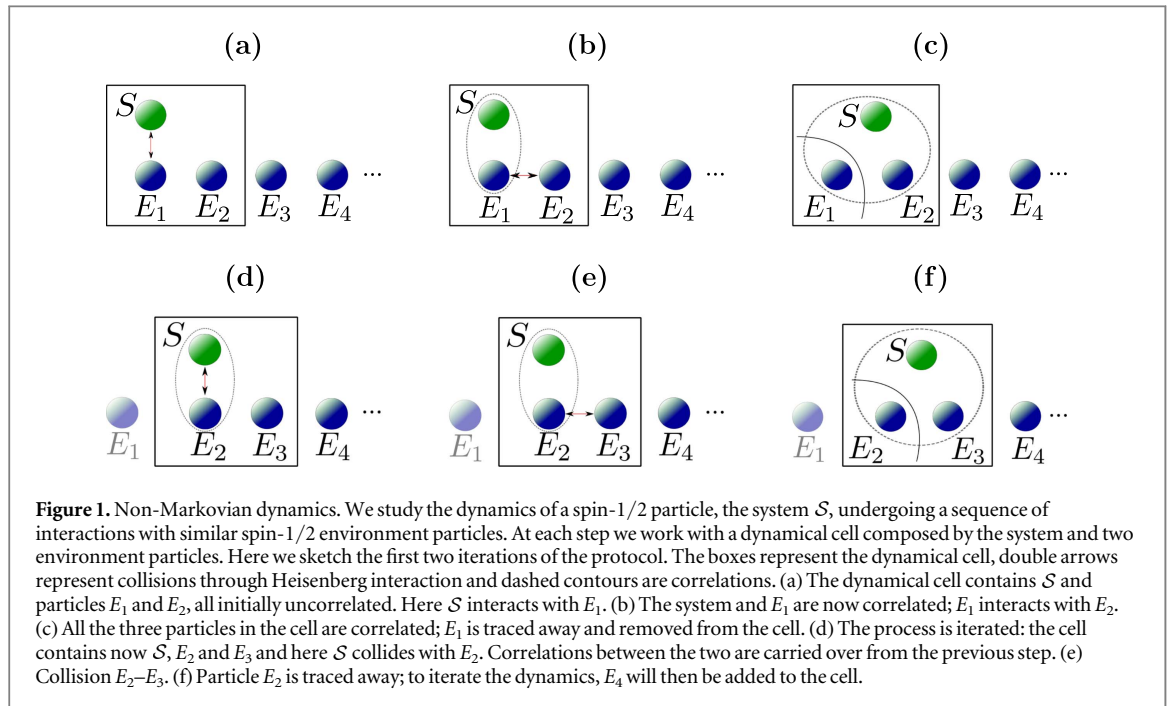
Marco Pezzutto^{1,2,3}, Mauro Paternostro³ and Yasser Omar^{1,2}¹ Instituto de Telecomunicações, Physics of Information and Quantum Technologies Group, Lisbon, Portugal² Instituto Superior Técnico, Universidade de Lisboa, Portugal³ Centre for Theoretical Atomic, Molecular and Optical Physics, School of Mathematics and Physics, Queen's University Belfast BT7 1NN, UKE-mail: marco.pezzutto@tecnico.ulisboa.pt**Keywords:** open quantum systems, collision-based models, quantum non-Markovianity, quantum thermodynamics, Landauer principle, quantum information**Abstract**

We study the dynamics of a spin-1/2 particle interacting with a multi-spin environment, modelling the corresponding open system dynamics through a collision-based model. The environmental particles are prepared in individual thermal states, and we investigate the effects of a distribution of temperatures across the spin environment on the evolution of the system, particularly how thermalisation in the long-time limit is affected. We study the phenomenology of the heat exchange between system and environment and consider the information-to-energy conversion process, induced by the system–environment interaction and embodied by the Landauer principle. Furthermore, by considering an interacting-particles environment, we tune the dynamics of the system from an explicit Markovian evolution up to a strongly non-Markovian one, investigating the connections between non-Markovianity, the establishment of system–environment correlations, and the breakdown of the validity of Landauer principle.

1. Introduction

Non-Markovian open-system dynamics has recently received considerable attention [1, 2], including the formulation of figures of merit for its characterization [3–8], and the first steps towards its experimental assessment [9–14]. While a full understanding of the origins of non-Markovianity [15, 16], and the formulation of a universal characterization of its implications are the objects of current investigations [17–21], the community interested in open system dynamics has recently recognised the relevance of non-Markovianity for the assessment of the properties of non-equilibrium quantum systems [22–25]. In particular, the role of memory effects (which are believed to be a key cause of the emergence of non-Markovian effects) in logically irreversible processes has recently attracted some attention [26, 27] in light of the relevance that Landauer principle has for information processing at both the classical and quantum level [28, 29, 34]. The relevance of the principle at the quantum scale has been largely debated, with contributions both at the theoretical [24, 26, 27, 30, 59, 32–35] and the experimental level [36–38].

In this work, we shed further light on the interplay between environmental memory effects and logical irreversibility in non-equilibrium processes. We construct a collisional model of the open-system dynamics of a spin-1/2 particle, of which figure 1 is an example, using and extending significantly a framework that was also used recently to investigate non-Markovianity [39, 40]. Our model consists of a sequence of discrete-time collisions, each ruled by a Heisenberg Hamiltonian, between the system and one environmental particle at a time. For non-interacting environmental particles all prepared in the same state, the system undergoes a homogenization dynamics [41]: in the long-time limit corresponding to a large number of collisions, the



system's state is asymptotically driven towards the initial preparation of the environmental particles.

Such homogenization is relatively robust against state fluctuations across the multi-particle environment induced, for instance, by a spatially inhomogeneous temperature.

For an environment of interacting particles, instead, the effective dynamics that the system undergoes can be tuned broadly from a fully Markovian to a highly non-Markovian regime. The crossover from Markovianity to non-Markovianity has long been object of investigation, both experimentally [42] and theoretically [43], with particular attention to non-Markovian effects due to a hierarchical environment [44, 45], the role of a non-Markovian memory-keeping environment in harnessing the quantum memory stored in a qubit [46, 47] and the ability to control the (non-)Markovian character of the dynamics of a composite system by tuning the internal couplings [48, 49].

In our study case, collisions occurring between environmental subsystems have a twofold effect: on the one hand, they induce system–environment correlations resulting in memory effects that allow the environment to retain information on the state of the system at previous steps of its discrete-time evolution; on the other hand, they enable a feedback process whereby information is coherently brought back into the state of the system, thus steering its state in a distinguished way with respect to the corresponding homogenization dynamics. We unveil the implications that such a rich dynamics has for logical irreversibility, assessing the break down of Landauer principle [28] as the non-Markovian character of the system's evolution is enhanced. In particular, we show a causal link between the system–environment correlations and the opening up of temporal *windows* in the time evolution of the system within which Landauer bound is no longer valid.

A connection between correlation revivals and non-Markovianity was also reported in [13, 54, 55], although in these works the authors investigate the dynamics of correlations within a composite system interacting with a local environment. Furthermore, it is worth mentioning that a breakdown of the II Law of Thermodynamics in the form of the Clausius inequality due to system–environment quantum correlations has also been evidenced in harmonic systems coupled to a bath of harmonic baths [56–58], and that in the context of generalizations of the II Law for systems strongly coupled to a reservoir, [59–61], the observed violations are only apparent.

The remainder of this work is structured as follows: in section 2 we summarize some key results on quantum non-Markovianity; in section 3 we introduce our collision model, its thermodynamics and the formulation of the Landauer principle for non-equilibrium quantum systems. Section 4 presents the results obtained with the fully Markovian dynamics, in particular the emergence of homogenization, while in section 5 we investigate the non-Markovian regime and show how non-Markovianity, local violations of the Landauer principle and correlations are causally connected. Section 6 draws our conclusions and presents some open questions that will be addressed in future works.

2. Quantum non-Markovianity

2.1. Definition and measure

The approach we use to define and measure quantum non-Markovianity, from [3], employs the *trace distance* [50] between two quantum states ρ_1 and ρ_2

$$D(\rho_1, \rho_2) := \frac{1}{2} \|\rho_1 - \rho_2\|, \quad \|\rho\| = \text{Tr} \sqrt{\rho^\dagger \rho}, \quad (1)$$

which is a metric in the space of density matrices. Two properties are particularly relevant: (a) the trace distance is a measure of the *distinguishability* between states and (b) it is *contractive* under positive trace preserving quantum dynamical maps, even if not completely positive. Let then $\{\Phi_t\}$ be a family of quantum dynamical maps, ρ_1 and ρ_2 two initial states and $\rho_{1(2)}(t) \equiv \Phi_t \rho_{1(2)}$ the corresponding evolved states. The dynamics given by the process Φ is *Markovian* if, for any pair of initial states, the trace distance $D(\rho_1(t), \rho_2(t))$ decreases monotonically for all $t \geq 0$. Conversely, a quantum dynamical process Φ is said to be *non-Markovian* if there exists a pair of initial states for which the trace distance between the evolved states is increasing in some time intervals. In other words, there exists two states ρ_1 and ρ_2 and some time $t \geq 0$ at which $\partial_t D(\rho_1(t), \rho_2(t))$ is strictly positive. A non-Markovian process can thus increase the distinguishability between two initially different states: the environment has some *memory effect* on the system dynamics. This fact can be used to quantify non-Markovianity. Denoting $\sigma(t) := \partial_t D(\rho_1(t), \rho_2(t))$, the *degree of non-Markovianity* \mathcal{N} of the quantum dynamical process Φ is

$$\mathcal{N}(\Phi) := \max_{\{\rho_1, \rho_2\}} \int_0^{+\infty} \frac{1}{2} (|\sigma(t)| + \sigma(t)) dt. \quad (2)$$

The integrand is non-null only in the intervals where the derivative is positive. Then a maximization over all pairs of initial states is performed, and it was shown in [51] that any two states maximising \mathcal{N} belong to the boundary of the state space and are orthogonal. Finally, as exposed in section 3, our dynamics is implemented in discrete time steps, therefore we compute the measure \mathcal{N} by substituting the derivative $\sigma(t)$ with the difference of the trace distance at steps n and $n-1$, $D(\rho_{1,n}, \rho_{2,n}) - D(\rho_{1,n-1}, \rho_{2,n-1})$.

2.2. Non-Markovianity and system–environment correlations

One important feature of the dynamics is the connection between system–environment correlations (hereafter referred to simply as *correlations*) and the manifestation of non-Markovianity. In [52] the authors provided a link between the behaviour of the derivative $\sigma(t)$ and system–environment correlations quantified by means of the matrix $\chi^{SE}(t) := \rho^{SE}(t) - \rho^S(t) \otimes \rho^E(t)$, in the form of an upper bound for $\sigma(t)$ depending explicitly on $\chi^{SE}(t)$. The result connects non-Markovianity with the emergent distinguishability between initially identical environment states, and with the creation of correlations. In that work, the authors provide the example of an $N+1$ spin-1/2 particle system, and find a connection between the time evolution of the trace distance and that of correlations, quantified by the *mutual information* between system and environment. Trace distance and correlations evolve in a periodic and synchronised fashion, both exhibiting a non-monotonic behaviour incompatible with a Markovian dynamics. A similar observation is reported in [39], and in our model we also observe this feature, as shown in section 5, and extend the connection between trace distance and correlations to include also the Landauer bound. In the work [53] a tighter connection between the trace distance derivative and correlations was provided, in the form of both an upper and a lower bound on $\sigma(t)$.

3. Dynamical model and thermodynamics

3.1. Basic setup and notation

The system and a generic environment particle are denoted by \mathcal{S} and \mathcal{E} respectively, and described by local spin-1/2 Hamiltonians

$$H_{S(E)} := \hbar \tilde{\omega}_{s(e)} \sigma_z / 2, \quad \tilde{\omega}_{s(e)} > 0. \quad (3)$$

The environmental particles are initially prepared in the thermal state $\rho_\beta := e^{-\beta H_E} / \mathcal{Z}$ at temperature T , where $\beta = 1/\kappa T$ is the inverse temperature and $\mathcal{Z} = \text{Tr}[e^{-\beta H_E}]$ is the corresponding partition function (we use units such that the Boltzmann constant κ takes value 1 from now on). As discussed in section 4, we allow for fluctuations in the preparation of the environmental particles. The choice of thermal states is consistent with the necessity of a well-defined temperature of the environment.

The dynamics proceeds through a sequence of interactions, or *collisions*, and we first consider a process in which the system interacts each time with a new environment particle, implementing the idea of a large, memoryless thermal bath. The system–environment interaction is ruled by the Heisenberg Hamiltonian and implemented through the unitary V_{SE}

$$H_{\text{int}} = \tilde{J}_{SE} (\sigma_x^S \sigma_x^E + \sigma_y^S \sigma_y^E + \sigma_z^S \sigma_z^E), \quad V_{SE} = \exp\left[-\frac{i}{\hbar} H_{\text{int}} \tau\right], \quad (4)$$

where τ is the interaction time. We call $H_0 = H_S + H_E$ the free Hamiltonian of system and environment, so that $U_0 = \exp(-\frac{i}{\hbar} H_0 \tau_0)$ gives the corresponding free evolution, occurring for a time τ_0 between two consecutive collisions. Starting with the environment particle in the pre-collision state $\rho_{\text{pre}}^E \equiv \rho_\beta$, the system is brought from step n to step $n + 1$ through the process

$$\rho_n^S \otimes \rho_{\text{pre}}^E \mapsto \rho_{n+1}^{SE} = U_0 V_{SE} (\rho_n^S \otimes \rho_{\text{pre}}^E) V_{SE}^\dagger U_0^\dagger, \quad (5)$$

and then the new marginal states $\rho_{n+1}^S = \text{Tr}_E[\rho_{n+1}^{SE}]$ and $\rho_{\text{post}}^E = \text{Tr}_S[\rho_{n+1}^{SE}]$ are computed.

3.2. Thermodynamics

From the marginal states we compute the von Neumann entropy $S_n = -\text{Tr}(\rho_n^S \ln \rho_n^S)$, the variation⁴ of the system energy and the exchanged heat at step n

$$\Delta U_n = \text{Tr}[H_S(\rho_n^S - \rho_{n-1}^S)], \quad \Delta Q_n = \text{Tr}[H_E(\rho_{\text{post}}^E - \rho_{\text{pre}}^E)]. \quad (6)$$

If $[H_{\text{int}}, H_0] \neq 0$ the interaction does not conserve the total energy of the physical system here at hand. The difference $W_n := \Delta Q_n - \Delta U_n$ can thus be interpreted as *work*, either poured into or extracted from the system by the unitary operation V_{SE} . The case of energy-conserving interactions is realized in the *resonance* condition $\tilde{\omega}_s = \tilde{\omega}_e$.

We can check the validity of the *Landauer bound* $\beta \Delta Q \geq \Delta S$ at each collision. In [27], the principle is given foundation in a framework of quantum statistical mechanics: we let $\Delta S = S_{n-1} - S_n$ be the entropy *decrease* of the system, and we call ΔQ the heat-exchange introduced in (6). The bound then holds if:

- (1) No other physical systems is involved;
- (2) The environment is initially in a thermal state;
- (3) The system and the environment are not initially correlated;
- (4) The dynamics proceeds through a joint unitary evolution.

We shall see in section 5 that inter-environment interactions, implemented as described below, can induce the presence of correlations between the system and an environmental particle before they interact directly, thus contradicting assumption (3) and allowing for violations of the bound.

3.3. Implementation of the non-Markovian dynamics

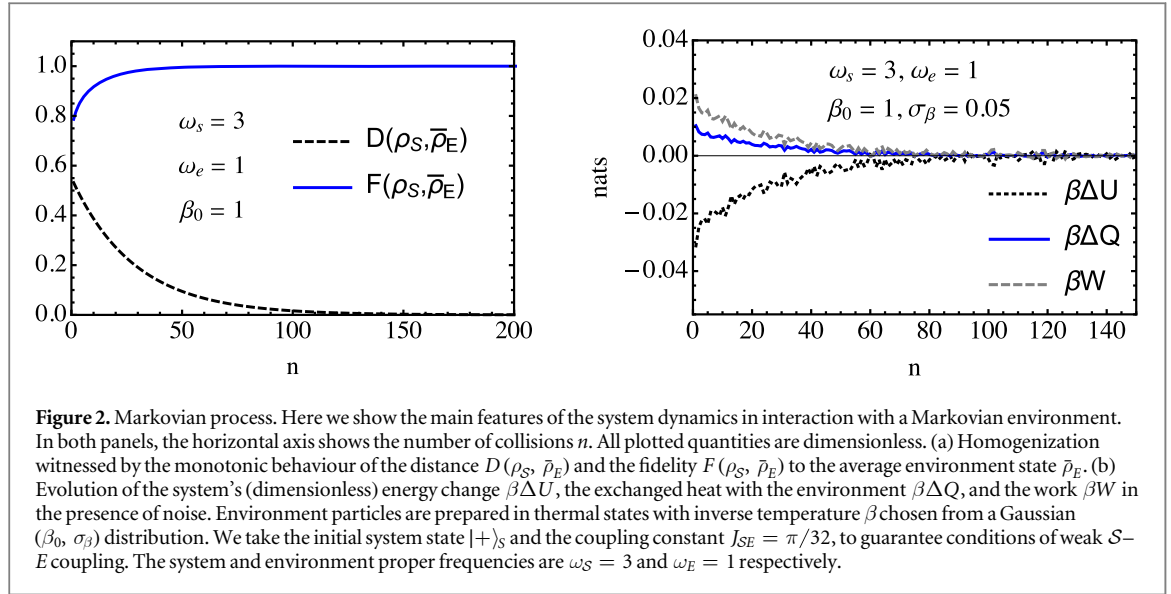
Let us now *switch on* the inter-environment interactions, which we alternate to the system–environment ones. The discrete-time evolution is achieved thanks to the iteration of a *dynamical cell* comprising the system and two environment particles. We now go through the n th iteration of the scheme, with reference to figure 1 exemplifying the first two steps. At the beginning, the dynamical cell contains \mathcal{S} , E_n and E_{n+1} . The \mathcal{S} – E_n collision occurs via the unitary operation V_{SE} in (5). From now on, we absorb the evolution times τ and τ_0 into the respective rates, so that we now consider dimensionless quantities such as $J_{SE} = \tilde{J}_{SE} \tau$, $\omega_{s,e} = \tilde{\omega}_{s,e} \tau_0$ and analogous ones. Then, E_n and E_{n+1} interact through a unitary operation V_{EE} similar to V_{SE} , where the dimensionless inter-environment coupling constant J_{EE} can be different from J_{SE} . The three particles in the dynamical cell can now be all correlated. The updated marginal states are computed, and thus the thermodynamical quantities. In particular, at each step we compute the marginal state of the environment particles before the \mathcal{S} – E_n and after the E_n – E_{n+1} interaction, and thus the exchanged heat $\Delta Q_n = \text{Tr}[(H_E \otimes H_E)(\rho_{E_n E_{n+1}}^{\text{post}} - \rho_{E_n E_{n+1}}^{\text{pre}})]$. In order to iterate the dynamics, E_n is now traced out, we compute the two-particle marginal state $\rho_{SE_{n+1}}^{\text{post}}$ and a fresh environmental particle E_{n+2} , prepared in the thermal state ρ_β , comes into the cell:

$$\rho_{SE_n E_{n+1}}^{\text{post}} \rightarrow \rho_{SE_{n+1}}^{\text{post}} \otimes \rho_\beta \equiv \rho_{SE_{n+1} E_{n+2}}^{\text{pre}}. \quad (7)$$

The whole process is then iterated.

One of our goals is to investigate the features of the dynamics from a fully Markovian to a completely non-Markovian regime, for which it is useful to express the operator V_{SE} in the form of a partial Swap, using the following result from [41]

⁴ Consistency between the information theoretical and the thermodynamical contexts bridged by the Landauer principle calls for choosing the natural logarithm, thus quantifying the entropy in *nats*.



$$e^{-i\frac{\phi}{2}} \exp \left[i\frac{\phi}{2} (\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z) \right] = e^{-i\phi} (\cos \phi \mathbb{I}_4 + i \sin \phi U_{sw}),$$

where U_{sw} is the two-particle Swap operator: $U_{sw}(|\psi_1\rangle \otimes |\psi_2\rangle) = |\psi_2\rangle \otimes |\psi_1\rangle$ for all $|\psi_1\rangle, |\psi_2\rangle$ in \mathbb{C}^2 . The partial Swap acts on any 2-particle state by leaving it unchanged with probability $\cos^2 \phi$ and swapping it with probability $\sin^2 \phi$. We can now write

$$V_{SE} = e^{-\frac{i}{\hbar} J_{SE}} [\cos(2J_{SE}) \mathbb{I}_4 + i \sin(2J_{SE}) U_{sw}], \quad (8)$$

and tune the operator from no interaction ($J_{SE} = 0$) up to a complete Swap ($J_{SE} = \pi/4$).

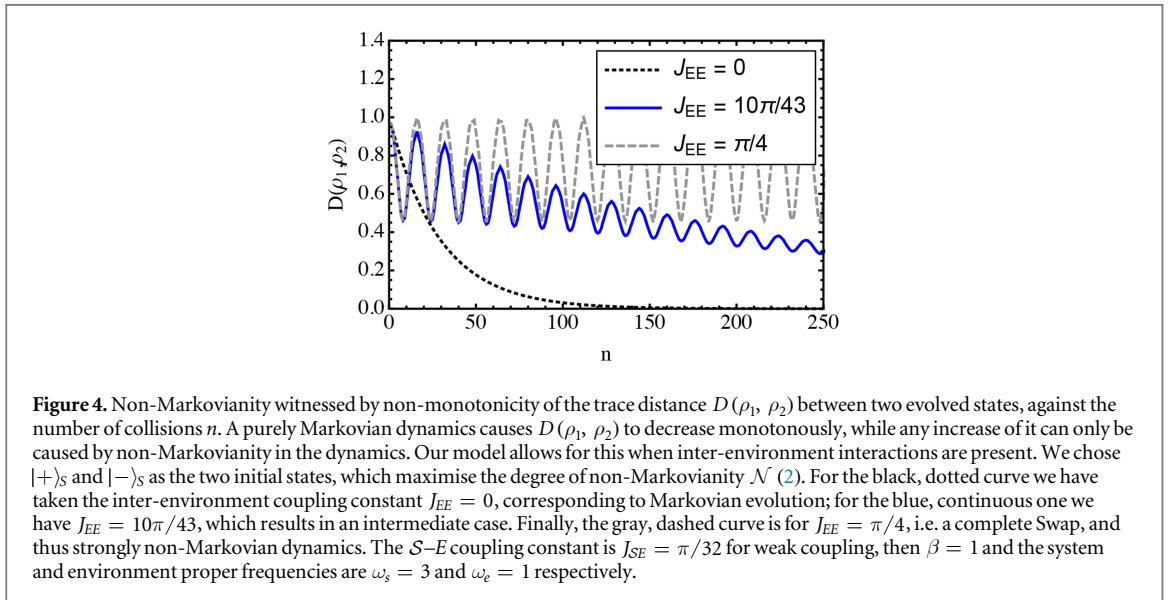
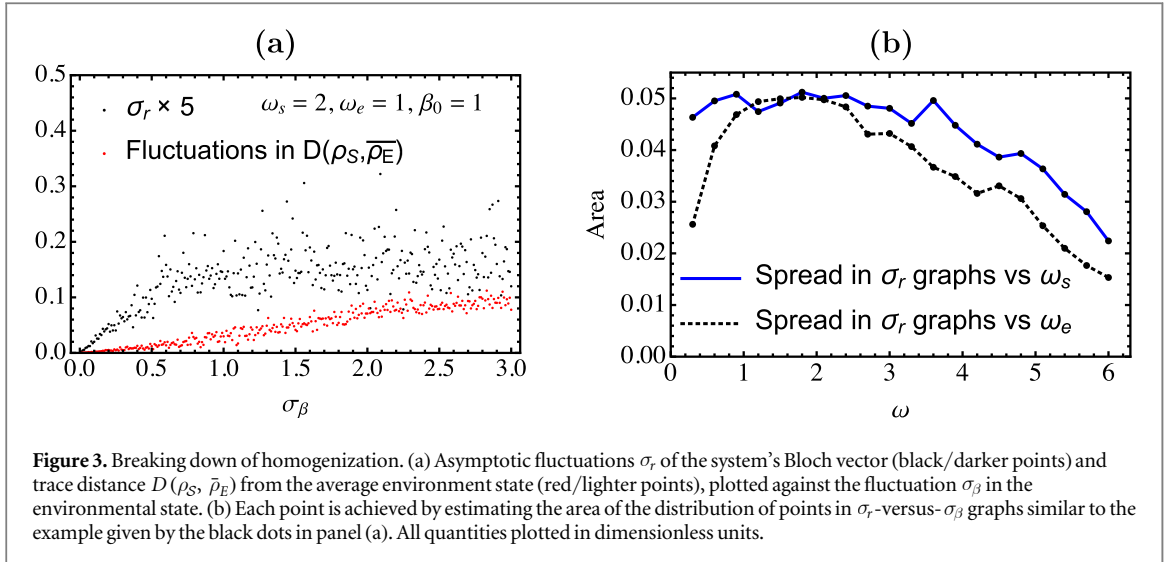
4. Observation of homogenization in the Markovian dynamics

Here we expose the results produced by the dynamics with no inter-environment interactions. If the environmental particles are all prepared in the same state ρ_β , the dynamics produces *homogenization*: the system reaches asymptotically the very same state in which the environment particles are prepared, $\rho_S \rightarrow \rho_\beta$ as illustrated in⁵ figure 2(a). This could appear to be counterintuitive at first, as one would expect the system to thermalize to the state $\exp[-\beta H_S]/\mathcal{Z}_S$. However, the dynamics is effectively governed by a global time-dependent Hamiltonian, and the system experiences an active *driving*. Homogenization occurs even for small fluctuations of the environmental states, as shown in figure 2(b). For each collision, we take β from a Gaussian distribution, centred in β_0 and with amplitude σ_β . We call $\bar{\rho}_E$ the average environmental state. The behaviour of the asymptotic fluctuations in the system appears to depend strongly on the entity of those occurring at the environment level. For small fluctuations in the environmental states, the asymptotic fluctuations increase almost linearly. However, for larger values of σ_β a less regular and more chaotic behaviour emerges, as shown in figure 3(a). Moreover, the quantitative trend followed by the system's fluctuations appear to depend strongly on the energy spacings ω_s and ω_e . In order to characterize such dependence and change of trend more quantitatively, we have estimated, through a Monte-Carlo approach, the area over which the cloud of points in figure 3(a) is distributed (see figure 3(b)). This provides an estimate of the *spread* of the distribution in the different dynamical situations that we have addressed. For small frequencies, the spread depends more heavily on ω_e than on ω_s , while for high frequencies it decreases in both cases. This effect is linked to the fact that, in such conditions, the interaction Hamiltonian becomes weaker than the free Hamiltonian. To summarise, the repeated interaction of the system with a Markovian environment produces homogenization, at least as far as the noise level in the environment is contained. For increasing noise, however, homogenization is lost and the asymptotic dynamics becomes less predictable.

5. Non-Markovianity, correlations and the Landauer bound

Here we present the results for the dynamics with interacting environment, up to the complete Swap between environmental particles. This case is equivalent to having the system interacting repeatedly with one single

⁵ Indeed, the equilibration condition $[H_{int}, \rho_S \otimes \rho_\beta] = 0$ is satisfied only if $\rho_S = \rho_\beta$.



environment particle. The asymptotic behaviour is the same as in the Markovian case, as non-Markovianity seems to affect only the transient before equilibration. The full Swap case embodies an exception: the system does not homogenize and the dynamics exhibits a periodic trend that is repeated indefinitely.

Figure 4 shows the trace distance between two different states evolving in time. In our case, the initial states that maximize the degree of non-Markovianity \mathcal{N} , given by (2), are $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$, up to a global phase factor. Figure 5 presents the behaviour of the Landauer bound formulated both in terms of the (discrete) flux $\beta\Delta Q$ and the change in entropy ΔS , and of the cumulative quantities

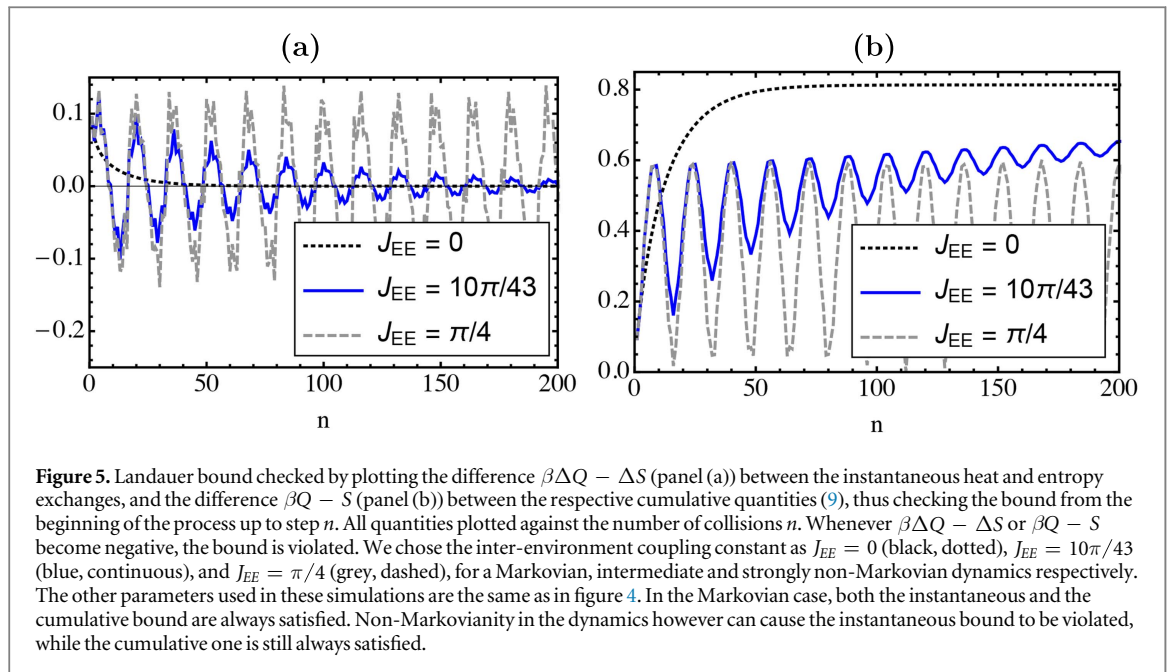
$$Q_n = \sum_{l=1}^n \Delta Q_l, \quad S_n = \sum_{l=1}^n \Delta S_l \equiv S(\rho_0^S) - S(\rho_n^S). \quad (9)$$

The negativity of $\beta\Delta Q_n - \Delta S_n$ implies the violation of the principle, which occurs repeatedly in the non-Markovian case. Such violation is closely connected to the presence of correlations between the system and E_n before their direct interaction. The *mutual information*

$$I(\rho_S, \rho_E) = S(\rho_S) + S(\rho_E) - S(\rho_{SE})$$

gives a measure of the correlations, whose presence is in explicit contradiction with one of the hypotheses behind the validity of the Landauer principle [27]. Nonetheless, the cumulative quantity $\beta Q_n - S_n$ remains positive at all times. Our analysis shows that the changes in entropy ΔS_n oscillate in time much more than $\beta\Delta Q_n$: such oscillations are responsible for the point-like violation of Landauer bound.

Figure 6 summarizes the main results of this work. At the beginning the dynamics is Markovian, then the interactions build up correlations which grow strong enough to cause a shift to the non-Markovian regime. As



the dynamics gets more and more non-Markovian and the trace distance increases, correlations diminish until they become negligible, at which point the dynamics returns within the Markovian regime, and the pattern repeats itself. The trace distance (discrete) derivative, the instantaneous Landauer bound and the (discrete) time derivative of mutual information proceed in a striking synchronous behaviour. The connection between $\beta\Delta Q - \Delta S$ and $\Delta I(\rho_S, \rho_E)$ can be understood intuitively as both are well approximated by the derivative of the von Neumann entropy S , the leading contribution to both in this parameter regime. However, a deeper and more complete theoretical explanation of our findings is still missing.

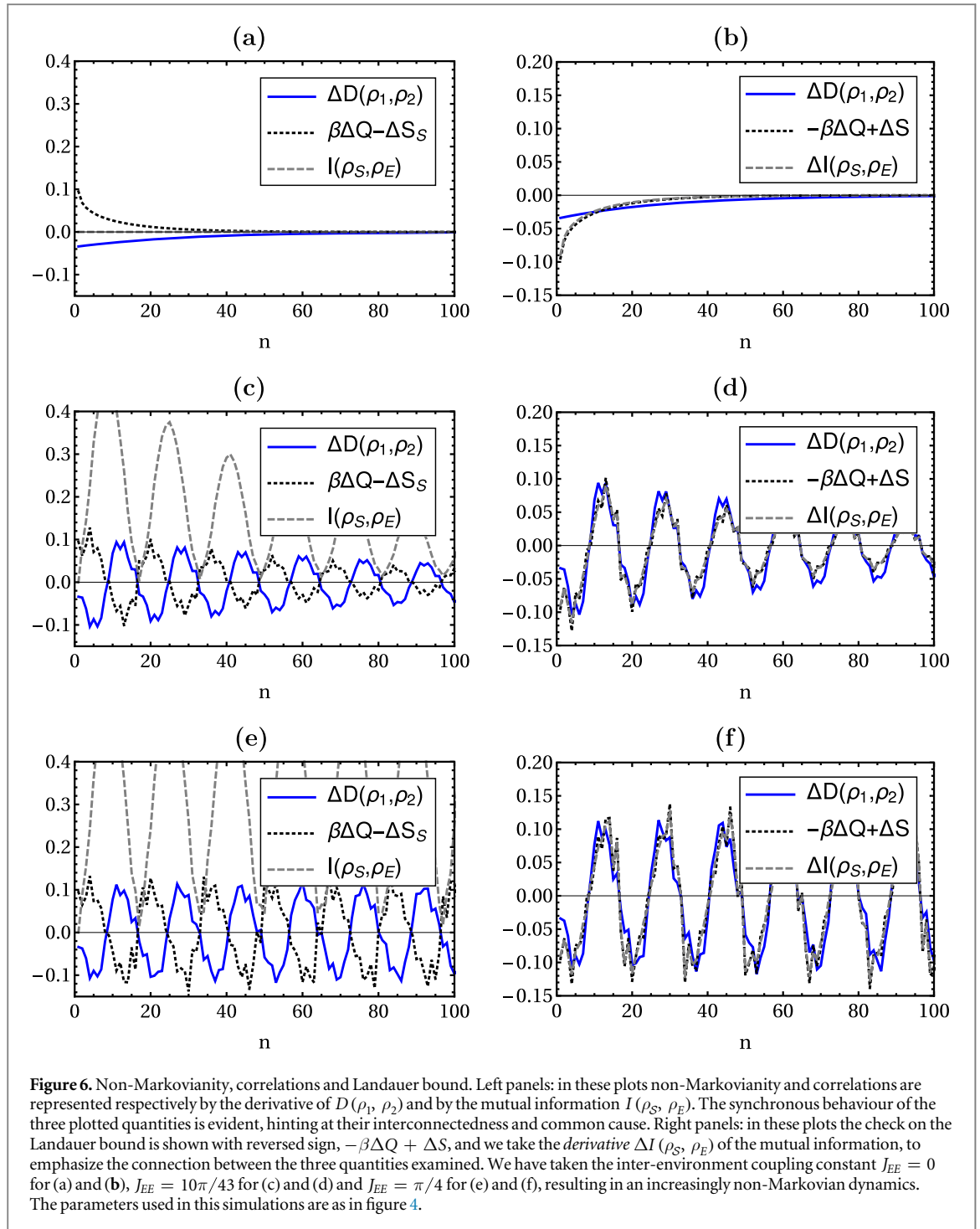
6. Concluding summary and remarks

We have studied the open-system dynamics undergone by a spin-1/2 particle through a sequence of discrete-time collisions with the elements of a spin environment. The asymptotic behaviour of the dynamics shows homogenization when the environmental particles are all in the same thermal state. This behaviour is maintained when the state of the environmental particles fluctuates weakly across their ensemble. For more significant fluctuations, however, homogenization is broken.

By allowing for inter-environment interactions, we have introduced memory effects in the dynamics of the system, which shows features of non-Markovianity. We have investigated the connection between the emergence of such behaviour, the creation of system–environment correlations, and the observed instantaneous violations of the Landauer bound for the system particle. The feedback of excitations from the environment to the system enabled by the inter-environment interactions results in the building up of system–environment correlations and invalidates one of the assumptions of the quantum formulation of Landauer principle, thus causing its break down. We observed a striking synchronous behaviour between the instantaneous emergence of non-Markovianity in the dynamics, the establishment of system–environment correlations and the mentioned violations of the Landauer bound. The three interconnected behaviours are clearly originated by a common origin, which will be the subject of our forthcoming investigations.

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