Role of correlations in the thermalization of quantum systems

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Abstract. We investigate the equilibration and thermalization properties of quantum systems interacting with a finite-dimensional environment. By exploiting the concept of time-averaged states, we introduce a completely positive map which allows us to describe in a quantitative way the dependence of the equilibrium state on the initial condition. Our results show that the thermalization of quantum systems is favored if the dynamics induces small system–environment correlations, as well as small changes in the environment, as measured by the trace distance.

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1. Introduction

The mechanisms behind thermalization have recently attracted renewed interest and initiated the development of novel statistical formulations of equilibration in the realm of quantum mechanics [1–9]. These descriptions have typically taken the total system under investigation as finite dimensional, so that the asymptotic limit of the dynamics does not exist and the system returns, with possibly very long recurrence time, arbitrarily close to its initial state infinitely many times [10, 11]. Relaxation to equilibrium in the usual sense is thus impossible. Nevertheless, one can introduce an extended notion of equilibration if the system tends towards some state, which can be identified as the equilibrium state of the dynamics, and stays close to it most of the time. There will still be some fluctuations around the equilibrium state, but extremely small or rare. It is important to note that extensions of these new approaches to the infinite-dimensional case have recently been developed [12].

In this work, we consider the situation in which a closed quantum system can be decomposed into two parts, an open system S and a bath B, and investigate the equilibration properties of the subsystem S. We use the extended notion of equilibration, i.e. we will say that the open system equilibrates if its time-evolved state (also called reduced state) $\rho_S(t)$ approaches some equilibrium state and spends most of the time close to it. In the same spirit, one can introduce the notion of thermalization of the open system by means of additional conditions on its equilibrium state [3]. Namely, one requires that the latter does not depend on the initial total state, besides a possible dependence on macroscopic parameters, such as temperature, characterizing the initial state of the bath. In this case one says that the open system thermalizes if, in addition, the equilibrium state takes the form of a Gibbs state. The capability of an open system to thermalize traces back ultimately to specific properties of the total Hamiltonian, which

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fixes the evolution of the total closed system and, in particular, characterizes the interaction
between the open system and the bath. Indeed, if the open system and the bath do not interact
no thermalization is expected. Moreover, if there are conserved quantities for the open system
its equilibrium state will unavoidably depend on the initial reduced state. More generally, it has
been shown [8] that the lack of a sufficient amount of entanglement in the energy eigenbasis is
a basic reason for the absence of thermalization.

Here, we want to discuss the thermalization of open quantum systems within the above-
mentioned framework, with the aim of clarifying the role of general dynamical mechanisms
that can induce or prevent it. Apart from the obvious situation of conserved quantities for the
open system, which features of the dynamics imply a dependence of the equilibrium state on the
initial reduced state? Thermalization requires a sufficient amount of entanglement in the energy
eigenbasis, but what is the role played by the interaction-induced correlations between the open
system and the bath? We investigate how the equilibrium state is modified when one resets
the correlations between the system and the bath, as well as the environmental state, to their
initial value. We find that small system–environment correlations, together with small changes
in the environmental state, generally lead to an equilibrium state that hardly depends on the
initial state of the open system. The system–environment correlations built by the dynamics thus
play a role which is, in a sense, contrary to that of the entanglement in the energy eigenbasis.
The interaction-induced correlations can prevent thermalization: strong system–environment
correlations and changes in the environmental state allow us to distinguish between equilibrium
states corresponding to different initial states. The information about the initial state of the
reduced system, transferred to the environment through the establishment of correlations, does
influence the equilibrium state. In this sense it can be considered as trapped in the equilibrium
state. For this reason, we will refer to this mechanism preventing thermalization as information
trapping. The quantitative characterization of information trapping will be given in terms of
trace distance, which measures the distinguishability between quantum states [13] and has
already been used to detect through its variation the information flow between the system and
the environment [19, 20], as also discussed later on.

2. General framework

Consider a finite-dimensional Hilbert space, which can be decomposed as $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$, with $\mathcal{H}_S$ and $\mathcal{H}_B$ Hilbert spaces associated with the open system $S$ and the bath $B$, respectively. A crucial assumption here is that the total Hilbert space $\mathcal{H}$ has finite dimension, which will be denoted by $d$, while we denote by $d_S$ and $d_B$ the dimensions of the open system and the bath. The evolution of the total system is governed by a one-parameter group of unitary operators $U(t) = e^{-\frac{i}{\hbar} H t}$, which is fixed by the total Hamiltonian

$$ H = H_S + H_B + H_{SB}, $$

where $H_S$ and $H_B$ are the free Hamiltonians of the system and the bath, and $H_{SB}$ is the interaction term. Given a total state $\rho_{SB}(t)$ at time $t$ we denote by $\rho_S(t) = \text{tr}_B \{ \rho_{SB}(t) \}$ the state of the open system, also called the reduced state, and by $\rho_B(t) = \text{tr}_S \{ \rho_{SB}(t) \}$ the state of the environment. If the initial total state factorizes, i.e. $\rho_{SB} = \rho_S \otimes \rho_B$ with a fixed initial state of the bath, there is a well-defined reduced dynamics [14], i.e. there is a family of completely positive and trace preserving maps $\Lambda(t)$ on the set $\mathcal{S}(\mathcal{H}_S)$ of statistical operators on $\mathcal{H}_S$ such that the reduced state
\[ \rho_S(t) \] at time \( t \) is given by \( \rho_S(t) = \Lambda(t) \rho_S \), where \( \rho_S \equiv \rho_S(0) \):
\[ \Lambda(t) : \mathcal{S}(\mathcal{H}_S) \rightarrow \mathcal{S}(\mathcal{H}_S), \]
\[ \rho_S \rightarrow \rho_S(t) = \Lambda(t) \rho_S, \]
with
\[ \Lambda(t) \rho_S = \text{tr}_B \left\{ U(t) \rho_S \otimes \rho_B U^\dagger(t) \right\}. \]

In [3], it has been shown that an open system equilibrates under very general assumptions if the effective dimension of the bath, i.e. the dimension of the subspace of \( \mathcal{H}_B \) involved in the dynamics, is much larger than the open-system dimension \( d_S \). In this case, for any initial state \( \rho_S \), the corresponding time-evolved state \( \rho_S(t) \) will be most of the time close to the time-averaged state \( \overline{\rho_S} \), which is defined as
\[ \overline{\rho_S} = \lim_{t \to \infty} \frac{1}{t} \int_0^t \text{d} \tau \rho_S(\tau) \]
and represents the equilibrium state of the reduced dynamics. Note that throughout the paper we will use an overline to denote the time average of any operator or function. More precisely, if the total Hamiltonian has non-degenerate energy gaps, the average distance between \( \rho_S(t) \) and the time-averaged state \( \overline{\rho_S} \) is bounded by [3]
\[ D(\rho_S(t), \overline{\rho_S}) \leq \frac{1}{2} \sqrt{\frac{d_S}{d_{\text{eff}}(\rho_B)}}, \]
where
\[ d_{\text{eff}}(\rho_B) = \frac{1}{\text{tr}_B \left\{ \rho_B^{-1} \right\}} \]
represents the effective dimension of the bath. Here and in the following, we characterize the distance between quantum states by means of the trace distance. Given two quantum states \( \rho^1 \) and \( \rho^2 \), their trace distance is defined as
\[ D(\rho^1, \rho^2) = \frac{1}{2} \| \rho^1 - \rho^2 \|, \]
where the trace norm is considered. The upper bound in (5), which has been proven in [3] for a pure product initial state, can be easily extended to a mixed product initial state, see appendix A.

On that account, the open system equilibrates under very general conditions, but nevertheless, despite some significant results [3, 5, 6, 8, 9], a widely open question still remains: what are the conditions determining whether an open system, besides equilibrating, also thermalizes? In the following, we will focus on this issue and, in particular, on finding the conditions for the dependence of the time-averaged state on the initial state of the open system.

3. Information trapping

3.1. Time-averaging map

First of all, let us take a closer look at the time-averaged state defined in (4). In the following, we assume for simplicity a non-degenerate Hamiltonian \( H = \sum_k E_k |E_k \rangle \langle E_k| \), but analogous considerations can be made in the degenerate case. For a fully generic initial total state \( \rho_{SB} \),
starting from equation (3) and by using the spectral resolution of the overall unitary time evolution operator, one has

$$\overline{\rho_S} = \sum_k \langle E_k | \rho_{SB} | E_k \rangle \sigma^k_S.$$  \hspace{1cm} (8)

The result is obtained exploiting the finite dimensionality of the total space; however, a possible extension to the infinite-dimensional case, in which the sum over \(k\) is replaced by a proper series, has been considered in [12]. In the expression for \(\overline{\rho_S}\) we have used the notation

$$\sigma^k_S \equiv \text{tr}_B \{ | E_k \rangle \langle E_k | \}. \hspace{1cm} (9)$$

If the initial total state is a product state \(\rho_S \otimes \rho_B\), with a fixed environmental state \(\rho_B\), equation (8) defines a map \(\Lambda\) on the state space of the open system \(\mathcal{S}(\mathcal{H}_S)\):

$$\rho_S \rightarrow \Lambda \rho_S := \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t \text{d} \tau \rho_S(\tau) = \sum_k \langle E_k | \rho_S \otimes \rho_B | E_k \rangle \sigma^k_S,$$  \hspace{1cm} (10)

which can also be written as

$$\Lambda \rho_S = \sum_k p_k \sigma^k_S,$$  \hspace{1cm} (11)

with

$$p_k \equiv \langle E_k | \rho_S \otimes \rho_B | E_k \rangle = \text{Tr} \{ | E_k \rangle \langle E_k | \rho_S \otimes \rho_B \}. \hspace{1cm} (12)$$

This map associates with any initial state of the system the corresponding time-averaged state, and therefore we will call it the time-averaging map. This is a linear, trace preserving and completely positive map and its image \(\Lambda(\mathcal{S}(\mathcal{H}_S)) = \text{Im} \Lambda\) can be identified as the set of equilibrium states of the reduced dynamics. A state \(\rho_S\) is said to be invariant if it is left unchanged by the time-averaging map, i.e. if \(\Lambda \rho_S = \rho_S\). A natural question then is whether equilibrium states are invariant, i.e. if, given a state \(\omega_S = \Lambda \rho_S\) for any initial state \(\rho_S\), one has \(\Lambda \omega_S = \omega_S\). This can happen for any \(\omega_S\) if and only if the map \(\Lambda\) is a projector. That is, it satisfies the idempotence relation \(\Lambda^2 = \Lambda\), where of course \(\Lambda^2\) indicates the composition of \(\Lambda\) with itself. Note that

$$\Lambda^2 \rho_S = \sum_{kk'} \langle E_k | \rho_S \otimes \rho_B | E_{k'} \rangle | E_{k'} \rangle \langle E_k | \sigma^k_S \otimes \rho_B | E_{k'} \rangle \sigma^{k'}_{S}.$$  \hspace{1cm} (13)

Let us now make the following important remark. First, recall that any trace preserving and positive map \(\Lambda\) is a contraction for the trace distance [15, 16], i.e. \(D(\Lambda \rho^1, \Lambda \rho^2) \leq D(\rho^1, \rho^2)\) for any \(\rho^1\) and \(\rho^2\). A map is further said to be strictly contractive [17, 18] if \(D(\Lambda \rho^1, \Lambda \rho^2) < D(\rho^1, \rho^2)\) for any \(\rho^1 \neq \rho^2\). Indeed, the time-averaging map \(\Lambda\) is contractive, but in general not strictly contractive. It is clear that the only way for it to be both strictly contractive and idempotent is to map every initial state to the same time-averaged state. That is, the maps \(\Lambda_\rho\), defined as

$$\Lambda_\rho \rho_S = \rho, \hspace{1cm} \forall \rho_S \in \mathcal{S}(\mathcal{H}_S) \hspace{1cm} (14)$$

for a fixed state \(\rho\), are the only idempotent and strictly contractive maps on \(\mathcal{S}(\mathcal{H}_S)\). In fact, let \(\omega_1, \omega_2 \in \text{Im} \Lambda\) be two elements of the image of \(\Lambda\), i.e. \(\omega_1 = \Lambda \rho^1_S\) and \(\omega_2 = \Lambda \rho^2_S\) for some \(\rho^1_S, \rho^2_S \in \mathcal{S}(\mathcal{H}_S)\). The idempotence of \(\Lambda\) implies that \(D(\Lambda \omega_1, \Lambda \omega_2) = D(\omega_1, \omega_2)\) and, because of the strict contractivity, it follows that \(\omega_1 = \omega_2\). Hence the image of \(\Lambda\) consists of only a single element which proves our claim.
As a consequence, the dependence of the equilibrium state on the initial state of the system can always be related to the violation of either property. In other words, the absence of thermalization can always be associated with either the lack of idempotence or strict contractivity of the time-averaging map. In the following we will focus on the violation of the idempotence of $\Lambda$, which will be referred to as information trapping. This will be shown to capture an interesting dependence of the equilibrium state on the initial state, and we will demonstrate a connection between information trapping and the creation of correlations between the system and the bath due to their mutual interaction.

### 3.2. Measure for information trapping

Rather than simply assessing whether the time-averaging map is idempotent, one needs to quantify its possible deviation from idempotence in order to point out if this can be treated as ‘small’. The very definition of the equilibration of a quantum system interacting with a finite-dimensional bath involves the idea that the reduced state $\rho_S(t)$ will stay most of the time in the neighborhood of the corresponding equilibrium state $\Lambda \rho_S$. For the sake of concreteness, let us denote by $\mathcal{X}$ the radius of such a neighborhood. Now, if the distance between two different equilibrium states $\Lambda \rho_S^1$ and $\Lambda \rho_S^2$ is smaller than $\mathcal{X}$, the corresponding time-evolved states $\rho_S^1(t)$ and $\rho_S^2(t)$ can be close to each other for almost all times, so that one cannot practically infer that they approach different equilibrium states by monitoring their evolution. This leads us to the conclusion that it is more meaningful to investigate the amount of information trapping of a given dynamics, rather than its mere presence.

In particular, we propose the following measure for information trapping:

$$ T(\Lambda) = \max_{\rho_S \in \mathcal{H}_S} D(\Lambda^2 \rho_S, \Lambda \rho_S). \tag{15} $$

This directly quantifies the violation of the idempotence of $\Lambda$, and it is indeed equal to 0 if and only if $\Lambda$ is idempotent. In appendix B, we introduce an alternative, but qualitatively equivalent, measure. Now, if $T(\Lambda)$ exceeds $\mathcal{X}$, there is some $\rho_S$ such that one can actually determine that $\rho_S$ and $\Lambda \rho_S$ evolve to different equilibrium states and no thermalization occurs. In addition, as will be shown by means of examples, the measure $T(\Lambda)$ provides a useful way to describe how the different features of a given dynamics can enhance or decrease the information trapping and thus the dependence of the equilibrium state on the initial state of the open system.

### 4. Information trapping and the system–environment correlations

In this section, we explicitly connect the notion of information trapping with the interaction-induced correlations between the system and the bath, as well as the changes in the environmental state. First of all, it is useful to come back to the full unitary dynamics, where the time averaging can be described by means of a trace preserving and completely positive map $U$, such that (compare with (8))

$$ U \rho_{SB} = \lim_{t \to \infty} \frac{1}{t} \int_0^t d\tau \rho_{SB}(\tau) = \sum_k \langle E_k | \rho_{SB} | E_k \rangle |E_k\rangle \langle E_k|. \tag{16} $$

Indeed, this map can be defined for any initial total state, but we will focus on the case $\rho_{SB} = \rho_S \otimes \rho_B$, with fixed $\rho_B$, to guarantee the existence of the reduced map $\Lambda$, which
can be expressed as
\[ \Lambda \rho_S = \text{tr}_B \{ U (\rho_S \otimes \rho_B) \}. \] (17)

In the following diagram, one can see the relation between the map \( U \) on the total system and both the reduced time-averaging map \( \Lambda \) and its twofold application \( \Lambda^2 \):

\[
\begin{array}{ccc}
\rho_S \otimes \rho_B & \xrightarrow{\tau} & \omega_{SB} = U (\rho_S \otimes \rho_B) \\
\downarrow & & \downarrow \\
\rho_S & \xrightarrow{\Lambda} & \omega_S = \Lambda \rho_S
\end{array}
\quad
\begin{array}{ccc}
\omega_S \otimes \rho_B & \xrightarrow{\tau} & U (\omega_S \otimes \rho_B) \\
\downarrow & & \downarrow \\
\omega_S & \xrightarrow{\Lambda} & \Lambda^2 \rho_S
\end{array}
\] (18)

where we introduced the notation \( \omega_{SB} = U (\rho_S \otimes \rho_B) \) to indicate the time-averaged state of the total system, so that \( \omega_S = \text{tr}_B \omega_{SB} = \rho_S \) and \( \omega_B = \text{tr}_S \omega_{SB} = \rho_B \) are the time-averaged states of the system and the bath, respectively. In particular, note how the reduced map \( \Lambda^2 \) is obtained after resetting the total state from \( \omega_{SB} \) to \( \omega_S \otimes \rho_B \). Now, the map \( U \) on the total state is always idempotent, i.e. \( U^2 = U \), as can be easily checked by means of (16), since it amounts to a von Neumann measurement of the total energy. Introducing the map \( \Phi = \text{tr}_B \circ U : \mathcal{S}(\mathcal{H}_S) \to \mathcal{S}(\mathcal{H}_S) \), from the diagram (18) and the idempotence of \( U \), one has \( \Lambda^2 \rho_S = \Phi (\omega_S \otimes \rho_B) \), while \( \Lambda \rho_S = \Phi (\omega_{SB}) \). But then, since \( \Phi \) is trace preserving and completely positive, the contractivity of the trace distance implies
\[ D(\Lambda^2 \rho_S, \Lambda \rho_S) \leq D(\omega_{SB}, \omega_S \otimes \rho_B) \leq D(\omega_{SB}, \omega_S \otimes \omega_B) + D(\rho_B, \omega_B). \] (19)

The information trapping is upper bounded by the total amount of correlations between the system and the bath in the total time-averaged state \( \omega_{SB} \) plus the distinguishability between the time-averaged state of the bath \( \omega_B \) and the fixed initial state \( \rho_B \). This means that, while a small amount of entanglement in the energy eigenbasis prevents a full thermalization [8], such a phenomenon will be generally favored if the dynamics builds up a small amount of correlations between the system and the bath, together with small changes in the state of the bath.

From a physical point of view, we can explain the connection between information trapping and system–environment correlations by taking advantage of the notion of information flow associated with the changes of the trace distance between reduced states in the course of time [19, 20]. The basic idea is that if there is some information trapped in the open system when it approaches the equilibrium, then, by resetting the system–environment correlations as well as the bath state to their initial condition, see (18), one can restart an information flow between the system and the bath, thus leading the system to a different equilibrium state. The distinguishability between the new equilibrium state \( \Lambda^2 \rho_S \) and \( \Lambda \rho_S \) then provides a way of quantifying the information trapped in the open system due to the system–environment correlations and the changes in the environmental state.

The relevance of bounds, determined by correlations in the total state as well as different environmental states, for the trace distance among different system states was first pointed out in [21], where the time dependence of the trace distance has been related to the presence of initial correlations. Here, however, the different system states do not correspond to different initial conditions, but rather to the action of distinct mappings.
5. Examples

5.1. Product energy eigenbasis

As a first representative example, consider a product energy eigenbasis \[ H = \sum_{k_1,k_2} E_{k_1k_2} |E_{k_1}\rangle \langle E_{k_1}| \otimes |E_{k_2}\rangle \langle E_{k_2}|. \] (20)

For such a Hamiltonian any reduced observable of the form \[ A = \sum_k a_k |E_k\rangle \langle E_k| \] represents a conserved quantity. Note that a non-degenerate conserved quantity on the open system implies a product eigenbasis of the total Hamiltonian. For \( H \) as in (20), the time-averaging map is not strictly contractive. In fact, one has

\[
\omega_S = \bar{\lambda}_S \rho_S = \sum_k \langle E_{k_1}| \rho_S |E_{k_1}\rangle |E_{E_{k_1}}\rangle \langle E_{E_{k_1}}|,
\] (21)

implying that if we choose as initial states two different elements of the basis \( \{|E_{k_1}\rangle\}_{k_1=1,...,d_S} \), \( \rho^1_S = |E_{j_1}\rangle \langle E_{j_1}| \) and \( \rho^2_S = |E_{l_1}\rangle \langle E_{l_1}| \), we obtain that

\[
D(\bar{\lambda}_S|E_{j_1}\rangle \langle E_{j_1}|, \bar{\lambda}_S|E_{l_1}\rangle \langle E_{l_1}|) = D(|E_{j_1}\rangle \langle E_{j_1}|, |E_{l_1}\rangle \langle E_{l_1}|) = 1.
\]

On the other hand, for a product energy eigenbasis there is no information trapping, since the time-averaging map is a projection. Even more, as is clearly evident from the expression of the time-averaged state (21), by setting \( \omega_S \otimes \rho_B \) as the initial total state, the reduced system does not evolve at all. This clearly shows that, unlike violation of strict contractivity, information trapping describes a mechanism preventing thermalization which is not only due to conserved quantities of the open system.

Moreover, for a product energy eigenbasis, the total time-averaged state is a product state, i.e. \( \omega_{SB} = \omega_S \otimes \omega_B \), but in general the time-averaged state of the bath \( \omega_B \) will be different from the initial state \( \rho_B \):

\[
D(\omega_B, \rho_B) = \frac{1}{2} \sum_{k_1 \neq k_2} \langle E_{k_1}| \rho_B |E_{k_2}\rangle |E_{E_{k_1}}\rangle \langle E_{E_{k_2}}| |E_{E_{k_1}}\rangle \langle E_{E_{k_2}}|.
\] (22)

Nevertheless, we have just now shown that \( \bar{\lambda}_S^2 \rho_S = \bar{\lambda}_S \rho_S \) for any \( \rho_S \), whatever the value of \( D(\omega_B, \rho_B) \) is in equation (22). Indeed, inequality (19) gives an upper bound to the amount of information trapping, which implies that it may so happen that, despite strong system–environment correlations or changes in the environmental state, the equilibrium state presents no information trapping.

5.2. The Jaynes–Cummings model

Let us now consider the Jaynes–Cummings model, i.e. a two-level system interacting under the rotating wave approximation with a single mode of the radiation field. Moreover, the latter is initially in a thermal state, so that the effective dimension of the bath can be made arbitrarily large by properly increasing the bath temperature. Indeed, this model is much simpler than systems with a macroscopic number of degrees of freedom [2, 5, 7] or many-body systems [22–25], which are usually taken into account when studying thermalization in the quantum setting. In this context, the Jaynes–Cummings model can be seen as a toy model, which allows us to explicitly evaluate all the quantities presented in the previous sections.
emphasize, however, that our general analysis can be applied to any open system, the only requirements being that the dimension of the total Hilbert space is finite and that the open system and the bath are initially uncorrelated.

The Hamiltonian giving the total dynamics is

\[ H = \omega_0 \sigma_+ + \omega b^\dagger b + g (\sigma_+ \otimes b + \sigma_- \otimes b^\dagger), \]

where \( \sigma_+ = |1 \rangle \langle 0 | \) and \( \sigma_- = |0 \rangle \langle 1 | \) are the raising and lowering operators of the two-level system, while the creation and annihilation operators of the field mode, \( b^\dagger \) and \( b \), obey the standard bosonic commutation relation. Finally, \( g \) is the coupling constant and we will denote by \( \Delta = \omega_0 - \omega \) the detuning between the frequency \( \omega_0 \) of the atom and the frequency \( \omega \) of the field mode. Moreover, one can think of a high-energy cutoff in order to keep the dimension of the bath finite. For an initial total state \( \rho_{SB} = \rho_S \otimes \rho_B \), where

\[ \rho_S = \begin{pmatrix} \rho_{11} & \rho_{10} \\ \rho_{01} & \rho_{00} \end{pmatrix}, \]

and \( \rho_B = e^{-\beta b^\dagger b}/Z \) is the thermal state of the bath, the reduced state at time \( t \) is given as

\[ \rho_S(t) = \begin{pmatrix} \rho_{00} (1 - \alpha(t)) + \rho_{11} \beta(t) & \rho_{10} \gamma(t) \\ \rho_{01} \gamma^*(t) & \rho_{00} \alpha(t) + \rho_{11} (1 - \beta(t)) \end{pmatrix}, \]

where

\[ \alpha(t) = \langle c^\dagger(\hat{n}, t)c(\hat{n}, t) \rangle_B, \]

\[ \beta(t) = \langle c^\dagger(\hat{n} + 1, t)c(\hat{n} + 1, t) \rangle_B, \]

\[ \gamma(t) = \langle c(\hat{n}, t)c(\hat{n} + 1, t) \rangle_B, \]

with \( \langle A \rangle_B = \text{Tr} \{ A \rho_B \} \), the number operator \( \hat{n} = b^\dagger b \) and

\[ c(\hat{n}, t) = e^{-\Delta t/2i} \left[ \cos \left( \sqrt{\Delta^2 + 4 g^2 \hat{n}} \frac{t}{2} \right) - \frac{i\Delta}{\sqrt{\Delta^2 + 4 g^2 \hat{n}}} \sin \left( \sqrt{\Delta^2 + 4 g^2 \hat{n}} \frac{t}{2} \right) \right]. \]

The time average can be directly calculated, thus giving

\[ \overline{\Lambda} \rho_S = \begin{pmatrix} \rho_{00} (1 - \bar{\alpha}) + \rho_{11} \bar{\beta} & 0 \\ 0 & \rho_{00} \bar{\alpha} + \rho_{11} (1 - \bar{\beta}) \end{pmatrix}, \]

with

\[ \bar{\alpha} = \left( \frac{\Delta^2 + 2 g^2 \hat{n}}{\Delta^2 + 4 g^2 \hat{n}} \right)_B, \]

\[ \bar{\beta} = \left( \frac{\Delta^2 + 2 g^2 (\hat{n} + 1)}{\Delta^2 + 4 g^2 (\hat{n} + 1)} \right)_B. \]

From (26) one has

\[ \overline{\Lambda}^2 \rho_S = \begin{pmatrix} \overline{\Lambda}^2 \rho_S \end{pmatrix}_{11} \begin{pmatrix} 0 \\ 0 \end{pmatrix} \]

\[ = \rho_{00} (1 - \bar{\alpha}) (\bar{\alpha} + \bar{\beta}) + \rho_{11} (1 + (\bar{\alpha} + \bar{\beta}) (\bar{\beta} - 1)), \]
so that $\Lambda^2 = \Lambda$ if and only if $\alpha + \beta = 1$ or $\alpha = 1$ and $\beta = 1$. The latter case corresponds to $g = 0$, which implies, as expected from the discussion in section 5.1, that there is no strict contractivity, see equation (25), and $\Lambda$ is idempotent. In all the other situations one has $\beta + \alpha - 1 < 1$ and the map is strictly contractive. Moreover, since for $\Delta \neq 0$, $\frac{\Delta^2 + 2\alpha^2 \beta}{\Delta^2 + 4 \alpha^2 \beta} + \frac{\Delta^2 + 2 \alpha^2 (\alpha + 1)}{\Delta^2 + 4 \alpha^2 (\alpha + 1)} > 1$, the only possibility to have $\alpha + \beta = 1$ is actually the resonant situation, $\Delta = 0$. In this case, the derivation of $\alpha$ through equation (27) has to be performed quite carefully. One can take the limit $\Delta \rightarrow 0$ into the function that the series in (27) converges to, or equivalently note that $\hat{c}\dagger(0, t)\hat{c}(0, t) = 1$, so that for $\Delta = 0$ one has

$$\alpha = \frac{1}{Z} + \sum_{n>0} \frac{1}{2} Z = \frac{1}{2Z} + \frac{1}{2},$$  

(29)

Thus, we have $\alpha + \beta - 1 = 1/(2Z)$, meaning that, apart from the trivial case, in this model there is always information trapping and there is never only one equilibrium state.

We can now characterize the dependence of the equilibrium state of the open system on its initial state by means of the measure for information trapping introduced in equation (15) of section 3.2:

$$T(\Lambda) = \max_{\rho \in \mathcal{B}} |\rho_{11}(\alpha + \beta - 2)(\alpha + \beta - 1) + (1 - \alpha)(\alpha + \beta - 1)|$$

$$= (\alpha + \beta - 1)(1 - \beta),$$

(30)

where the maximum is assumed for $\rho_S = |1\rangle \langle 1|$. Note that from (29) one has for $\Delta = 0$

$$T(\Lambda) = \frac{1}{4} (1 - e^{-\beta \omega}).$$

(31)

In figure 1, we have plotted the measure $T(\Lambda)$ as a function of the detuning $\Delta$, for different values of the bath temperature $T$. The resonant situation $\Delta = 0$ represents a minimum for the dependence of the equilibrium state on the initial state. The residual amount of information trapping has to be compared with the radius of equilibration $\mathcal{X}$, as discussed in section 3.2. If $T(\Lambda) < \mathcal{X}$, the residual dependence of the equilibrium state on the initial state of the open system is not enough to recognize that $\rho_S$ and $\Lambda^t \rho_S$ evolve to different equilibrium states. On the grounds of numerical simulations, we can consider the rhs of (5) as an upper bound to $\mathcal{X}$, see also [8]. Thus, in figure 1 one can see that the information trapping is actually larger than $\mathcal{X}$ for high enough detuning.

From the point of view of the Hamiltonian eigenvectors, the condition $\Delta = 0$ is in fact very peculiar: the eigenvectors of the Jaynes–Cummings Hamiltonian, the so-called dressed states, reduce for $\Delta = 0$ to

$$|\Psi_{n}^{\pm}\rangle = \frac{1}{\sqrt{2}} (|0, n\rangle \pm |1, n - 1\rangle),$$

(32)

plus the vacuum state $|0, 0\rangle$. Every eigenvector $|\Psi_{n}^{\pm}\rangle$ is maximally entangled in $\mathbb{C}_{n}^2 \otimes \mathbb{C}_{n}^2$, where $\mathbb{C}_{n}^2$ is the two-dimensional subspace of $\mathcal{H}_B$ spanned by $|n\rangle$ and $|n - 1\rangle$. Note that, at resonance, both the entanglement on the energy eigenbasis and the amount of residual information trapping, see (31), do not depend on the coupling constant $g$ between the system and the bath. Thus, for the model at hand, a high entanglement in the energy eigenbasis ensures an (effective) independence of the equilibrium state from the initial state of the open system, as one can expect from [8].

New Journal of Physics 14 (2012) 113034 (http://www.njp.org/)
Figure 1. Measure for information trapping $\mathcal{T}(\Lambda)$ defined in (30) as a function of $\Delta/\omega$ for $g/\omega = 1$ and $\beta\omega = 0.003$ (blue line), $\beta\omega = 0.005$ (red line) and $\beta\omega = 0.01$ (yellow line); the values for $\Delta = 0$ can be obtained through equation (31), as well. The marks on the vertical axis give the values of the rhs of (5), which are upper bounds for the value of $\mathcal{X}$ as discussed in the text, for $\Delta = 0$ and for the different temperatures: these marks are, respectively, 0.027, 0.035 and 0.050.

Figure 2. Measure for information trapping $\mathcal{T}(\Lambda)$ (blue line) and $D(\omega_{SB}, \omega_{S} \otimes \omega_{B}) + D(\omega_{B}, \rho_{B})$ (red, dashed line) versus $\Delta/\omega$ for $g/\omega = 1$ and $\beta\omega = 0.01$; $\omega_{SB}$ is given by $U(\rho_{S} \otimes \rho_{B})$, see (18), with $\rho_{B} = e^{-\beta\omega \hat{n}}/Z$ and $\rho_{S} = |1\rangle\langle 1|$ the reduced state maximizing the information trapping in (30).

Now, we want to explicitly quantify the role of the system–environment correlations, as well as the changes in the environmental state, by means of the upper bound introduced in (19), i.e. $D(\omega_{SB}, \omega_{S} \otimes \omega_{B}) + D(\omega_{B}, \rho_{B})$. This quantity can be explicitly evaluated by following the same strategy employed in [27] to calculate the amount of correlations in the total Gibbs state, which takes advantage of the block diagonal structure of the total Hamiltonian (23) with respect to the dressed states. In figure 2, one can see the measure $\mathcal{T}(\Lambda)$ as a function of the detuning $\Delta$ compared with the upper bound. We observe how the latter, despite being quite far from the
actual value of the measure for information trapping, follows its behavior from a qualitative point of view. Indeed, as follows from the bound (19), small system–environment correlations and changes in the state of the bath imply a small amount of information trapping, and therefore an equilibrium state of the two-level system that hardly depends on its initial state. But for the model at hand, whenever strict contractivity holds, we have in addition that the more the interaction induces system–environment correlations and changes in the environmental state, the more the equilibrium state will depend on the initial reduced state $\rho_S$.

5.3. Structured environment

As a complementary example, we consider now the model of a system interacting with a structured reservoir introduced in [28, 29]. A two-level system is coupled to two energy bands with the same width $\delta \varepsilon$; the energy levels in each band are equidistant and there are $N_1$ ($N_2$) levels in the lower (upper) band. The distance $\Delta E$ between the central levels of the two bands is in resonance with the free energy of the two-level system. The coupling constants between the two-level system and the two bands are independent and identically distributed complex Gaussian random variables and their overall strength is parameterized by a constant $\lambda$. Finally, we assume that the initial state of the environment is given by a maximally mixed combination of the lower band levels. Thus, by means of Hilbert space averaging [29] or correlated projection superoperator [30] techniques, one obtains the following equations in the Schrödinger picture for the excited state population $\rho_{11}(t)$ and the coherence $\rho_{10}(t)$:

$$\dot{\rho}_{11}(t) = -\gamma \rho_{11}(t) + \gamma_1 \rho_{11}(0),$$
$$\dot{\rho}_{10}(t) = -(i\Delta E + \gamma_2/2)\rho_{10}(t),$$

where $\gamma_i = 2\pi\lambda^2 N_i/\delta \varepsilon$, $i = 1, 2$, and $\gamma = \gamma_1 + \gamma_2$. These equations are solved by

$$\rho_S(t) = \begin{pmatrix} \rho_{11} e^{-\gamma_1 t} + \gamma_2 e^{-\gamma_2 t} & \rho_{10}(-\gamma_2/2 + i\Delta E) \\ \rho_{01} e^{-\gamma_2 t} - i\Delta E & \rho_{00} - \rho_{11}(\gamma_2/2 e^{-\gamma_2 t} - 1) \end{pmatrix}. \quad (34)$$

The time-averaging map corresponding to the evolution in (34) is, see (10),

$$\Lambda \rho_S = \begin{pmatrix} \rho_{11} & 0 \\ \rho_{00} + \rho_{11}(1 - \gamma_1/\gamma) \end{pmatrix}. \quad (35)$$

Indeed, for $\gamma_2/\gamma_1 = 0$ this map reduces to the identity map, while in all other situations it is a strictly contractive non-idempotent map. The square of the time-averaging map is given by

$$\Lambda^2 \rho_S = \begin{pmatrix} \rho_{11} & 0 \\ \rho_{00} + \rho_{11}(1 - \gamma_1/\gamma) \end{pmatrix}, \quad (36)$$

so that the measure for information trapping defined in (15) is

$$T(\Lambda) = \frac{\gamma_1}{\gamma} - \frac{\gamma_1^2}{\gamma^2} = \frac{N_1 N_2}{(N_1 + N_2)^2} \quad (37)$$

and the maximization is obtained with $\rho_S = |1\rangle \langle 1|$. The information trapping is completely determined by the ratio $N_1/N_2$ and, in particular, it vanishes only in the limit $N_2/N_1 \to 0$, which corresponds to the trivial situation $\Lambda = 1$, or in the limit $N_1/N_2 \to 0$. 

New Journal of Physics 14 (2012) 113034 (http://www.njp.org/)
Finally, let us present a remark about the connection between information trapping and the non-Markovianity of a quantum dynamics [19, 31]. Note that the relation between the asymptotic state of a reduced dynamics and its non-Markovianity has been studied in [32]. From (34) one can easily obtain a time-local master equation in the form
\[
\frac{d}{dt} \rho(t) = K(t) \rho(t) \quad (38)
\]
to characterize the dynamics of the two-level system. The time-local generator \( K(t) \) is, in fact, simply given as [26]
\[
K(t) = \dot{\Lambda}(t) \Lambda^{-1}(t), \quad (39)
\]
so that, for the model at hand, it reads
\[
\frac{d}{dt} \rho(t) = -i \Delta E \left[ \sigma_+ \sigma_- \rho(t) \right] + \Gamma_1(t) \left[ \sigma_- \rho(t) \sigma_+ - \frac{1}{2} \{ \sigma_+ \sigma_- \rho(t) \} \right]
\]
\[
+ \Gamma_2(t) \left[ \sigma_z \rho(t) \sigma_z - \rho(t) \right], \quad (40)
\]
with
\[
\Gamma_1(t) = \frac{\gamma_2^{\gamma}}{\gamma_1 e^{\gamma t} + \gamma_2}, \quad \Gamma_2(t) = \frac{\gamma_1 \gamma_2}{4} \left( 1 - e^{-\gamma t} \right). \quad (41)
\]
Such coefficients are positive at every time, implying that the reduced dynamics under consideration is always Markovian, both in the sense that it implies a monotonic decrease of the trace distance in the course of time and in the sense that it is fixed by a divisible family of dynamical maps [19, 31, 33, 34]. This clearly shows that one can actually have information trapping also in the presence of a Markovian dynamics: more generally, the dependence of the equilibrium state of the open system on its initial state does not provide a signature of non-Markovianity according to the above-mentioned definitions.

6. Conclusions

In this paper, we have investigated the thermalization of finite-dimensional quantum systems, within the framework of the theory of open quantum systems. By only assuming an initial product state, we have shown how one can introduce a time-averaging map on the state space of the open system that associates with any initial state the corresponding equilibrium state. In this way, we could formulate relevant questions related to equilibrium properties of the open system in terms of suitable properties of the time-averaging map. In particular, the dependence of the equilibrium state on the initial reduced state can always be traced back to the violation of at least one of the properties of strict contractivity and idempotence of the time-averaging map. Indeed, the violation of idempotence has been shown to provide an indication of the amount of information about the initial system state stored in the equilibrium state. We have therefore dubbed this violation as information trapping. It has been shown to be strictly connected to the interaction-induced correlations between the system and the bath, as well as the changes in the environmental state, which keep track of the system–environment information flow. More precisely, small system–environment interactions, together with small changes in the state of the bath, lead to an equilibrium state with a small dependence on the initial state of the open system, as quantified by means of the trace distance.
Furthermore, we have introduced a measure in order to evaluate the amount of information trapping of a given dynamics. This provides a way to determine how different features of the dynamics influence the dependence of the equilibrium state on the initial state of the open system and therefore how they can favor or prevent a full thermalization. In particular, in the Jaynes–Cummings model one can conclude that if the time-averaging map is strictly contractive, then strong system–environment correlations and changes in the environmental state imply a significant dependence of the equilibrium state on the initial state of the open system. Indeed, it would be important to determine whether, or at least to what extent, this implication holds in general.

Finally, let us note that the present results could provide a further insight into the role of the weak coupling assumption in the process of thermalization. If the open system and the bath are weakly coupled, one expects that the total state at a generic time can be effectively described by neglecting the system–environment correlations and the changes in the environmental state. In this regard, it will be of interest to investigate the connection between the correlation properties of the total time-averaged states studied in this work and the correlation properties of the total state in the course of time.

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Appendix A. Extension of the bound in the average distance between a state and its time average to a generic initial product state

Here we prove inequality (5) for a generic initial product state $\rho_S \otimes \rho_B$, under the assumption that the total Hamiltonian $H$ has non-degenerate energy gaps, i.e. $E_k - E_{k'} = E_j - E_{j'}$ implies that $k = k'$ and $j = j'$ or $k = j$ and $k' = j'$. We will essentially follow the proof in [3] for initial pure product states. First, let us introduce the notation

$$c_{kk'} = \langle E_k | \rho_S \otimes \rho_B | E_{k'} \rangle,$$

so that

$$\rho_S(t) = \sum_{kk'} e^{-i(E_k - E_{k'})t} c_{kk'} \text{tr}_B \{|E_k\rangle\langle E_k|\},$$

and therefore, compared with equations (8) and (9),

$$\overline{\Delta}_S \rho_S = \sum_k c_{kk} \text{tr}_B \{|E_k\rangle\langle E_k|\}.$$

New Journal of Physics 14 (2012) 113034 (http://www.njp.org/)
From the bound $\|\rho\| \leq \sqrt{d_\mathcal{S}} \|\rho\|_{HS}$, where $\| \cdot \|_{HS}$ denotes the Hilbert–Schmidt norm $\|A\|_{HS}^2 = \text{tr}_\mathcal{S} A^\dagger A$, and by exploiting the concavity of the square root we have

$$D(\rho_S(t), \overline{\Lambda}_\rho) \leq \frac{1}{2} \sqrt{d_\mathcal{S} \text{tr}_\mathcal{S} \{ (\rho_S(t) - \overline{\Lambda}_\rho)^2 \}}.$$  \hfill (A.4)

From equations (A.2) and (A.3), it follows that

$$\rho_S(t) - \overline{\Lambda}_\rho = \sum_{k \neq k'} e^{-i(E_k - E_{k'}) t} c_{kk'} \text{tr}_\mathcal{B} \{ |E_k\rangle \langle E_k'| \}.$$  

Using the identity

$$\text{tr}_\mathcal{S} \{ \text{tr}_\mathcal{B} \{ |E_k\rangle \langle E_k'| \} \text{tr}_\mathcal{B} \{ |E_k'\rangle \langle E_k'\rangle \} \} = \text{tr}_\mathcal{B} \{ |E_k\rangle \langle E_k| \} \text{tr}_\mathcal{S} \{ |E_k'\rangle \langle E_k'| \} ,$$

and the fact that $H$ has non-degenerate energy gaps, one finds that

$$\text{tr}_\mathcal{S} \{ (\rho_S(t) - \overline{\Lambda}_\rho)^2 \} = \sum_{k \neq k'} c_{kk'} c_{k'k} \text{tr}_\mathcal{B} \{ |E_k\rangle \langle E_k| \} \text{tr}_\mathcal{S} \{ |E_k'\rangle \langle E_k'| \} \}
\leq \sum_{k \neq k'} c_{kk'} c_{k'k} \text{tr}_\mathcal{B} \{ |E_k\rangle \langle E_k| \} \text{tr}_\mathcal{S} \{ |E_k'\rangle \langle E_k'| \} .$$

Further exploiting the Schwarz inequality

$$c_{kk'} c_{k'k} \leq c_{kk} c_{k'k} ,$$  \hfill (A.5)

we finally come to

$$\text{tr}_\mathcal{S} \{ (\rho_S(t) - \overline{\Lambda}_\rho)^2 \} \leq \sum_{k \neq k'} c_{kk} c_{k'k} \text{tr}_\mathcal{B} \{ |E_k\rangle \langle E_k| \} \text{tr}_\mathcal{S} \{ |E_k'\rangle \langle E_k'| \} \}$$

$$= \text{tr}_\mathcal{B} \left\{ \sum_{k} c_{kk} \text{tr}_\mathcal{S} \{ |E_k\rangle \langle E_k| \} \sum_{k'} c_{k'k} \text{tr}_\mathcal{S} \{ |E_k'\rangle \langle E_k'| \} \right\}$$

$$= \text{tr}_\mathcal{B} \left\{ \rho_B(t)^2 \right\} ,$$  \hfill (A.6)

which, together with (A.4) and (6), gives (5).

**Appendix B. An alternative measure for information trapping**

The measure for information trapping in equation (15) directly quantifies the effect of removing correlations and resetting the environmental state to its initial condition in the time-averaged state $\omega_{SB}$, see also (18) and (19). On the other hand, it is in some sense arbitrary to consider only the twofold application of the time-averaging map instead of a large number of applications. It is, in fact, clear that the dynamics obtained by resetting the total state to $\overline{\Lambda}_\rho \otimes \rho_B$ can still present some information trapped in the new equilibrium state as a consequence of further system–environment correlations built up by the interaction, and so on. For this reason, we introduce the following alternative measure for information trapping:

$$T_\infty(\overline{\Lambda}) = \max_{\rho_S \in \mathcal{S}(\mathcal{H}_S)} D \left( \lim_{k \to \infty} \overline{\Lambda}_\rho, \overline{\Lambda}_\rho \right) ,$$  \hfill (B.1)

which is set equal to 1 if the limit does not exist for some $\rho_S$. It is important to note that the two measures, $T(\overline{\Lambda})$ and $T_\infty(\overline{\Lambda})$, give the same qualitative characterization of information trapping,
i.e. also $T_{\infty}(\Lambda)$ is equal to 0 if and only if $\Lambda$ is idempotent. The ‘if’ part is obvious. To check the ‘only if’ part, $T_{\infty}(\Lambda) = 0$ implies by definition the existence of the limit in (B.1), and therefore in particular
\[
\lim_{k \to \infty} \| \Lambda^k \rho_S - \Lambda^{k-1} \rho_S \| = 0, \quad \forall \rho_S \in \mathcal{S}(\mathcal{H}_S). \tag{B.2}
\]
Moreover, we can define the map $\overline{\Lambda}$ through $T_{\infty}(\Lambda) = 0$ implies by definition the existence of the limit in (B.1), and therefore in particular
\[
\lim_{k \to \infty} \| \Lambda^k - \Lambda^{k-1} \rho_S \| = 0, \quad \forall \rho_S \in \mathcal{S}(\mathcal{H}_S).
\]
Furthermore, note that if $\Lambda$ is strictly contractive, due to the Banach fixed point theorem it has a unique invariant state $\rho^0_S = \lim_{k \to \infty} \Lambda^k \rho_S$, which is then a natural reference state to quantify the dependence of the equilibrium state on the initial condition: in this case, measure (B.1) can be simply written as
\[
T_{\infty}(\Lambda) = \max_{\rho_S \in \mathcal{S}(\mathcal{H})} D(\rho^0_S, \Lambda \rho_S). \tag{B.3}
\]
For example, in the Jaynes–Cummings model, for $g \neq 0$, the time-averaging map $\Lambda$ (26) is strictly contractive. Since
\[
(\Lambda^r \rho_S)_{11} = (1 - \alpha) \sum_{l=0}^{r-1} (\beta + \alpha - 1)^l + \rho_{11} (\beta + \alpha - 1)^r, \tag{B.4}
\]
the limit map $\overline{\Lambda}^\infty$ is given by
\[
\overline{\Lambda}^\infty \rho_S = \begin{pmatrix}
\frac{1-\alpha}{2-\beta-\alpha} & 0 \\
0 & \frac{1-\alpha}{2-\beta-\alpha}
\end{pmatrix}, \tag{B.5}
\]
which then provides the unique invariant state of the strictly contractive map $\Lambda$. The measure (B.1) is thus given by
\[
T_{\infty}(\Lambda) = \frac{\alpha + \beta - 1}{2 - \beta - \alpha} (1 - \beta), \tag{B.6}
\]
and the measure for information trapping reads
\[
T_{\infty}(\Lambda) = \frac{N_1}{N_1 + N_2}, \tag{B.7}
\]
to be compared with (37). In both cases the use of this alternative measure does not qualitatively change the results, which justifies concentrating on idempotence.
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