From Pure Schrödingerian to Statistical Dynamics

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Abstract

Many processes in nature seem to be entirely controlled by transition rates and the corresponding statistical dynamics. Some of them are in essence quantum, like the decay of excited states, the tunneling through barriers or the decay of unstable nuclei. Thus, starting from first principles, those systems should be analyzed on the basis of the Schrödinger equation. In the present paper we consider a two level system coupled to an environment which is basically described by an two-band energy scheme. For appropriately tuned environment parameters, the excitation probability of the two level system exhibits statistical dynamics, while the full system follows the coherent, unitary pure state evolution generated by the Schrödinger equation.

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1. Introduction

Quite naturally the question for the decay behavior of quantum states is not new and thus there is a considerable amount of theories aiming in that direction.

First of all Fermi's Golden Rule should be mentioned, a formula of enormous practical importance. Nevertheless its derivation is based on the assumption of a short perturbation and thus in can hardly account for a full, continuous decay process, all the way down to equilibrium.

The decay process associated with the spontaneous emission of an atom is described by the Weisskopf Wigner Theory in a way that is not based on a short perturbation. But this theory describes particularly an atom coupled to the electromagnetic field in the vacuum state and is thus hard to generalize to arbitrary environments in arbitrary states.

In the context of the system-environment scenario there are also the theories based on quantum master equations. Most of them involve some projection operator technique as well as the Born approximation and typically systems must be Markovian [1]. Many derivations are based on an initial state which is a product state with a thermal bath part. Some derivations even assume this structure for the full relaxation process [2,3]. This assumption is often backed up by the argument that since for no interaction no system-environment correlations could be generated, weak interactions (Markovicity) could only generate negligible correlations [4,5]. Furthermore, since those master equations result in maps on the considered system of the form \( \dot{\rho}(t + \tau) = M(\tau) \rho(t) \) that allow for an itera-
tion as $\mathcal{M}(\tau_1 + \tau_2) = \mathcal{M}(\tau_1)\mathcal{M}(\tau_2)$ [6], the final state with regard to one map might be the initial state with regard to another. This fact also seems to support the idea that at least weak interactions could not produce considerable correlations.

In the following we thus shortly comment on the question of relaxation and correlations in general, and then introduce an alternative theory of the relaxation process that takes arbitrary pure, possibly correlated or even entangled full system states into account.

### 2. Relaxation and Correlations

Is it possible that a full bi-partite system (system-reservoir-model) undergoes a unitary transformation, such that the purity of the considered system decreases (entropy increases, relaxation), without substantial system-reservoir correlations being generated?

This question shall be addressed within this section. To those ends we specify the “correlations”, $\hat{\rho}$ as an addend of the full system density matrix, $\hat{\rho}$:

$$\hat{\rho}_c := \hat{\rho} - \hat{\rho}_s \otimes \hat{\rho}_r \quad (\hat{\rho}_s := \text{Tr}_r \{ \hat{\rho} \}, \hat{\rho}_r := \text{Tr}_s \{ \hat{\rho} \})$$

(1)

Obviously $\hat{\rho}_s \otimes \hat{\rho}_r$ specifies the uncorrelated product part of the density matrix. To measure the “size” of the correlated and the uncorrelated parts we use the absolute value, $P_c$, of an operator:

$$P_x := \sqrt{\text{Tr} \{ \hat{\rho}_x^2 \}} \quad x = s, r, \text{none}$$

(2)

Evidently $P_x$ is also the purity of the corresponding (sub)system. To decide whether or not correlations are negligible we finally want to consider the “correlations/product” coefficient $\eta$:

$$\eta := \frac{P_c}{P_s P_r}$$

(3)

If $\eta \ll 1$, correlations may safely be neglected.

Computing the size of the correlations yields:

$$P_c^2 = P_s^2 - 2\text{Tr} \{ \hat{\rho}_s \hat{\rho}_r \} + P_s^2 P_r^2$$

(4)

Since the trace of a product of two hermitian matrices fulfills the conditions on an inner product, one finds through application of Schwartz’ s inequality:

$$|\text{Tr} \{ \hat{\rho}_s \hat{\rho}_r \} | \leq PP_s P_r$$

(5)

Inserting this into (4) yields:

$$P_c^2 \geq (P - P_s P_r)^2$$

(6)

or for the coefficient $\eta$

$$\eta \geq \frac{P}{P_s P_r} - 1$$

(7)

$P$ is invariant under unitary transformation. Often the reservoir is assumed to be exactly stationary which might not precisely hold true, nevertheless $P_r(0) \approx P_r(t)$ should be a reasonable approximation for large reservoirs. Thus the only quantity that may substantially change upon relaxation on the right hand side of (7) is $P_s$. And if $P_s$ decreases, $\eta$ obviously increases. For the case of a stationary bath and an initial product state one finds

$$\eta \geq \frac{P_s(0)}{P_s(t)} - 1$$

(8)

This lower bound on $\eta$ may easily take on rather high values, e.g., for an $N$-level system coupled to a bath in the high temperature limit ($kT$ much larger than the level spacing) one gets for an initially pure state, $P_s(0) = 1$,

$$\eta \geq \sqrt{N} - 1$$

(9)

This result is absolutely independent of the interaction strength. It only connects a decrease of purity (increase of entropy) to an increase of system-reservoir correlations, regardless of the timescale on which this relaxation process happens. Thus we conclude that, quite contrary to the idea of system and bath remaining uncorrelated correlations are generically generated upon relaxation.

### 3. The Hilbert Space Average Method

The method of describing the relaxation process we are going to present here relies on a step-wise solution of the Schrödinger equation. Naturally, this approach, like all other approaches, relies on approximations.

The crucial approximation here is the replacement of some specific quantities by their Hilbert space averages. Hilbert space averages are averages of quantities defined as functions of the pure full system state, over sets of such states which share a crucial common feature, like, e.g., in our case, the same excitation probability for the considered system. If the distribution of excitation probabilities among the states of the respective set is broad, the replacement of an actual value by its Hilbert space average will most likely be a bad
approximation. If the distribution is tightly centered around its mean value, the replacement still only represents a “best unbiased guess” but with distributions getting narrower, this guess obviously gets better and better. In our case there is evidence that the width of the distribution vanishes with an increasing number of environment states.

Based on this idea we derive a rate equation, that describes the decay which is controlled only by the Schrödinger equation, up to some fluctuations.

4. The System-Environment Model

The energy scheme of the situation we are going to analyze is depicted in Fig. 1. A two level system, g (“gas”), is in contact with a “many level” environment or “container”, c {We use this nomenclature for purely historical reasons [7]. Only the relevant parts of the spectrum of the environment enter the model. These are, in this case, two “bands” of width \( \delta \epsilon \), containing \( N^c_1 \) \( (N^c_0) \) equidistant eigenstates in the upper (lower) band. Therefore the level spacing within the upper (lower) energy “band” is

\[
\Delta E^c_1 := \frac{\delta \epsilon}{N^c_1} \quad \text{and} \quad \Delta E^c_0 := \frac{\delta \epsilon}{N^c_0}.
\]

In the following, quantities of the “upper band” of the environment get the subscript 1, whereas quantities of the “lower band” get the subscript 0. If we, e.g., consider an evolution from an initial state, with the system in the excited state \( |1\rangle \) and the environment in the “lower band”, 0, due to overall energy conservation the only other set of states that the full system can evolve into, is the set with the considered system in the ground state \( |0\rangle \) and the environment in its “upper band”, 1. The Hamiltonian within the relevant subspace of the entire Hilbert space may thus be organized as follows,

\[
\hat{H} = \begin{pmatrix}
\ddots & 0 & \hat{V} \\
0 & \ddots & 0 \\
\hat{V} & 0 & \ddots \\
\end{pmatrix}
\]

\[
|\psi^{ex}\rangle \quad |\psi^{gr}\rangle
\]

| | g | container c |
|---|---|---|
| [1] | \( \delta \epsilon \) \( N^c_1 \) |
| [0] | \( \delta \epsilon \) \( N^c_0 \) |

Fig. 1. Discrete two-level system coupled to a quasi-continuous container system. This set-up exhibits, for a sufficiently high state density in the container system, and an adequately tuned coupling, an exponential decay of an excitation in the gas system.

where \( i \) \( (j) \) count the levels in the upper (lower) “band” of the environment. The Hamiltonian is displayed in the eigenbasis of the uncoupled system, for simplicity we assume for the moment that the coupling \( \hat{V} \) only adds terms to the Hamiltonian in the off-diagonal blocks. This corresponds to an coupling which may give raise to energy exchange between the subsystems.

We now introduce two projectors, which project out the upper (lower) part of the state of the system

\[
\hat{P}^{ex} := |1\rangle \langle 1| \otimes 1^c, \quad \hat{P}^{gr} := |0\rangle \langle 0| \otimes 1^c,
\]

(12)

where \( 1^c \) is the 1-operator in the environmental system. In the following we call that part of the wave vector that corresponds to the considered system in the excited state \( |\psi^{ex}\rangle \) and the part that corresponds to the system in the ground state \( |\psi^{gr}\rangle \), i.e.,

\[
|\psi^{ex}\rangle := \hat{P}^{ex} |\psi\rangle, \quad |\psi^{gr}\rangle := \hat{P}^{gr} |\psi\rangle
\]

\[
\Rightarrow |\psi\rangle = |\psi^{ex}\rangle + |\psi^{gr}\rangle.
\]

Note that neither \( |\psi^{ex}\rangle \) nor \( |\psi^{gr}\rangle \) are normalized individually.

To analyze this model we first transform to the Dirac or interaction picture [8]

\[
\hat{U}(t, 0) := \hat{U}_0 := e^{-\frac{i}{\hbar}H_0 t}, \quad |\psi_1\rangle := \hat{U}_0^\dagger |\psi\rangle, \quad \hat{V}_1 := \hat{U}_0^\dagger \hat{V} \hat{U}_0,
\]

(14)

where \( H_0 \) is the Hamiltonian of the uncoupled system. The Schrödinger equation in this representation reads

\[
\frac{i \hbar}{\partial t} |\psi\rangle = \hat{V}_1 |\psi\rangle,
\]

(15)

where both states and operators are now time-dependent, i.e. also \( \hat{V}_1 \) is a time dependent operator, but preserves the off-diagonal block form as before.

The crucial quantities in the context of a decay to equilibrium are the probabilities to find the system in
its exited (ground) state, $W^{\text{ex}}(W^{\text{gr}})$. Due to the diagonality of $\hat{H}_0$, those quantities have the same representation in the interaction as well as in the Schrödinger picture,

$$
W^{\text{ex}} = \langle \psi^{\text{ex}}_1 | \psi^{\text{ex}}_1 \rangle = \langle \psi^{\text{ex}}_1 | \psi^{\text{ex}}_1 \rangle
t
W^{\text{gr}} = \langle \psi^{\text{gr}}_1 | \psi^{\text{gr}}_1 \rangle = \langle \psi^{\text{gr}}_1 | \psi^{\text{gr}}_1 \rangle.
$$

For simplicity we omit in the following the interaction picture subscript ‘I’, but all the following considerations refer to this picture.

5. Time Evolution

To approximate the evolution of the system for a short time step, we can truncate the corresponding Dyson series

$$
|\psi(\tau)\rangle \approx \left(1 - \frac{i}{\hbar} \hat{U}_1(\tau) - \frac{1}{\hbar^2} \hat{U}_2(\tau)\right) |\psi(0)\rangle.
$$

This is a truncation of second order, in which the $\hat{U}$’s are the time ordered integrals that occur in the Dyson series [8]

$$
\hat{U}_1(\tau) = \int_0^\tau d\tau' \hat{V}(\tau') ,
$$

$$
\hat{U}_2(\tau) = \int_0^\tau d\tau' \hat{V}(\tau') \int_0^{\tau'} d\tau'' \hat{V}(\tau'').
$$

According to the hermiticity of $\hat{V}(\tau)$, $\hat{U}_1(\tau)$ should be hermitian too, which is not the case for $\hat{U}_2(\tau)$. $\hat{U}_1(\tau)$ has the same off-diagonal form as $\hat{V}(\tau)$ whereas $\hat{U}_2(\tau)$ has here a block diagonal form according to the interaction matrix. (To further simplify notation we do not write the $\tau$ dependence of the $\hat{U}$’s explicitly. Furthermore, we omit the time dependence of the wave function, if it refers to the initial state, i.e., $|\psi(0)\rangle := |\psi\rangle$).

As mentioned above we are interested in the time evolution of the probability to find the system in its excited state $W^{\text{ex}}(\tau)$, or ground state $W^{\text{gr}}(\tau)$, respectively. Initially we consider $W^{\text{ex}}(\tau)$. Neglecting all terms of higher than second order (products of $\hat{U}_1$ and $\hat{U}_2$ as well as terms proportional to $\hat{U}_2^2$) and taking the special off-diagonal block form of the interaction into account, we get from (17) and (13)

$$
W^{\text{ex}}(\tau) = \langle \psi^{\text{ex}}_1 | \psi^{\text{ex}}_1 \rangle + \frac{i}{\hbar} \langle \psi^{\text{ex}}_1 | \hat{U}_1 | \psi^{\text{ex}}_1 \rangle
$$

- $\frac{i}{\hbar} \langle \psi^{\text{ex}}_1 | \hat{U}_1 | \psi^{\text{ex}}_1 \rangle$

$$
+ \frac{1}{\hbar^2} \langle \psi^{\text{ex}}_1 | \hat{U}_1^2 | \psi^{\text{ex}}_1 \rangle - \frac{1}{\hbar^2} \langle \psi^{\text{ex}}_1 | (\hat{U}_2 + \hat{U}_1^2) | \psi^{\text{ex}}_1 \rangle.
$$

$tion, if it refers to the initial state, i.e.,

$$
W^{\text{gr}}(\tau) = \langle \psi^{\text{gr}}_1 | \psi^{\text{gr}}_1 \rangle + \frac{i}{\hbar} \langle \psi^{\text{gr}}_1 | \hat{U}_1 | \psi^{\text{gr}}_1 \rangle
$$

- $\frac{i}{\hbar} \langle \psi^{\text{gr}}_1 | \hat{U}_1 | \psi^{\text{gr}}_1 \rangle$

$$
+ \frac{1}{\hbar^2} \langle \psi^{\text{gr}}_1 | \hat{U}_1^2 | \psi^{\text{gr}}_1 \rangle - \frac{1}{\hbar^2} \langle \psi^{\text{gr}}_1 | (\hat{U}_2 + \hat{U}_1^2) | \psi^{\text{gr}}_1 \rangle.
$$

The strict overall probability conservation requires

$$
W^{\text{ex}}(\tau) + W^{\text{gr}}(\tau)
$$

$$
= \langle \psi^{\text{ex}}(\tau) | \psi^{\text{ex}}(\tau) \rangle + \langle \psi^{\text{gr}}(\tau) | \psi^{\text{gr}}(\tau) \rangle
$$

$$
= \langle \psi^{\text{ex}}_1 | \psi^{\text{ex}}_1 \rangle + \langle \psi^{\text{gr}}_1 | \psi^{\text{gr}}_1 \rangle = 1.
$$

Since the normalization is already fulfilled in the zero order, all higher orders must vanish. Obviously the first order vanishes automatically. Thus, exploiting (21), for the second order of the sum of (19) and (20) we find

$$
\langle \psi^{\text{gr}}(\tau) | \hat{U}_2 + \hat{U}_1^2 | \psi^{\text{ex}} \rangle = \langle \psi^{\text{gr}}_1 | \hat{U}_2 + \hat{U}_1^2 | \psi^{\text{ex}}_1 \rangle,
$$

$$
\langle \psi^{\text{gr}}(\tau) | \hat{U}_2 + \hat{U}_1^2 | \psi^{\text{gr}} \rangle = \langle \psi^{\text{gr}}_1 | \hat{U}_2 + \hat{U}_1^2 | \psi^{\text{gr}}_1 \rangle.
$$

Inserting this into (19) and (20) yields

$$
W^{\text{ex}}(\tau) = \langle \psi^{\text{ex}}_1 | \psi^{\text{ex}}_1 \rangle + \frac{i}{\hbar} \langle \psi^{\text{ex}}_1 | \hat{U}_1 | \psi^{\text{ex}}_1 \rangle
$$

- $\frac{i}{\hbar} \langle \psi^{\text{ex}}_1 | \hat{U}_1 | \psi^{\text{ex}}_1 \rangle$

$$
+ \frac{1}{\hbar^2} \langle \psi^{\text{ex}}_1 | \hat{U}_1^2 | \psi^{\text{ex}}_1 \rangle - \frac{1}{\hbar^2} \langle \psi^{\text{ex}}_1 | (\hat{U}_2 + \hat{U}_1^2) | \psi^{\text{ex}}_1 \rangle.
$$

$$
W^{\text{gr}}(\tau) = \langle \psi^{\text{gr}}_1 | \psi^{\text{gr}}_1 \rangle + \frac{i}{\hbar} \langle \psi^{\text{gr}}_1 | \hat{U}_1 | \psi^{\text{gr}}_1 \rangle
$$

- $\frac{i}{\hbar} \langle \psi^{\text{gr}}_1 | \hat{U}_1 | \psi^{\text{gr}}_1 \rangle$

$$
+ \frac{1}{\hbar^2} \langle \psi^{\text{gr}}_1 | \hat{U}_1^2 | \psi^{\text{gr}}_1 \rangle - \frac{1}{\hbar^2} \langle \psi^{\text{gr}}_1 | (\hat{U}_2 + \hat{U}_1^2) | \psi^{\text{gr}}_1 \rangle.
$$

For an exact evaluation of the right hand side one would need to know the $|\psi^{\text{ex}}_1\rangle, |\psi^{\text{gr}}_1\rangle$ in detail. But rather than doing so, we replace now the actual quantities by their corresponding Hilbert space averages, according to the approximation scheme explained in sect.3. The appropriate set of states over which the average has to be taken here is the set of all states featuring the same excitation probability $\langle \psi^{\text{ex}}_1 | \psi^{\text{ex}} \rangle$. Some justification for this replacement has been given in sect.3, some comes from the numerical results, sect. 9, and for full detailed justification, see [9,10]. Since not only the justification of the replacement but also the actual computation of the respective are beyond
the scope of this text we again refer the interested reader to [9,10]. Here, we only want to give and discuss the results:

\[
\begin{align*}
[\langle \psi_1^{ex}|\bar{U}_i|\psi_1^{ex}\rangle] &= [\langle \psi_1^{ex}|\bar{U}_i|\psi_2^{ex}\rangle] = 0, \quad (25) \\
[\langle \psi_1^{ex}|\bar{U}_i^2|\psi_2^{ex}\rangle] &= \frac{\langle \psi_1^{ex}|\psi_2^{ex}\rangle}{N_0^2} \text{Tr}_{ex}\{\bar{U}_i^2\}, \\
[\langle \psi_1^{ex}|\bar{U}_i^2|\psi_1^{ex}\rangle] &= \frac{\langle \psi_1^{ex}|\psi_2^{ex}\rangle}{N_1^2} \text{Tr}_{gr}\{\bar{U}_i^2\},
\end{align*}
\]

where \([\ldots]\) denotes the Hilbert space average and Tr_{ex(gr)}\{\ldots\} the trace over the upper (lower) subspace of the operator.

Plugging those results into (23), we get

\[
\begin{align*}
W^{ex}(\tau) &= W^{ex}(0) + \frac{W^{gr}(0)}{\hbar^2 N_0^2} \text{Tr}_{gr}\{\bar{U}_i^2\} - \frac{W^{ex}(0)}{\hbar^2 N_0^2} \text{Tr}_{ex}\{\bar{U}_i^2\}, \\
W^{gr}(\tau) &= W^{gr}(0) + \frac{W^{ex}(0)}{\hbar^2 N_0^2} \text{Tr}_{ex}\{\bar{U}_i^2\} - \frac{W^{gr}(0)}{\hbar^2 N_1^2} \text{Tr}_{gr}\{\bar{U}_i^2\}.
\end{align*}
\]

Now we have to analyze those traces in more detail. We will do this explicitly for the upper subspace but by simply exchanging the indices, the result will be valid for the lower subspace as well

\[
\text{Tr}_{ex}\{\bar{U}_i^2\} = \sum_{j=1}^{N_0^2} (j|\bar{U}_i^2|j) = \sum_{j=1}^{N_0^2} |\bar{U}_i|j)^2. \quad (27)
\]

Here \(j\) runs over the eigenstates of \(\hat{H}_0\) in the upper subspace (note this corresponds to the lower “band” of the environment). The object that is summed over here is evaluated in the literature in the context of Fermi’s Golden Rule,

\[
\left|\bar{U}_i\right|^2 = \sum_{i=1}^{N_0^2} |i|\bar{V}_i|j)^2 \frac{4\sin^2(\frac{i\omega_{i,j}\tau}{\hbar})}{\omega_{i,j}}. \quad (28)
\]

with

\[
\omega_{i,j} = \frac{1}{\hbar} (E_j - E_i) = \frac{1}{\hbar} (j\Delta E^*_i - i\Delta E_i^*), \quad (29)
\]

see Fig. 3(a).

6. The Linear Regime

Our arguments, including the conditions we have to impose on the model, follow now closely the ones brought forth in the context of Fermi’s Golden Rule.

The summation in (28) consists of two different terms: the transition elements of the interaction matrix and a weight \(f(\omega)\). The spacing of different \(\omega_{i,j}\) is given by

\[
\Delta \omega = \omega_{i,j} - \omega_{i+1,j} = \frac{\Delta E_i}{\hbar} = \frac{\delta \epsilon}{N_0^2 \hbar}, \quad (30)
\]

where we have used (10). The function

\[
f(\omega) = \frac{\sin^2(\frac{i\omega\tau}{\hbar})}{\omega^2} \quad (31)
\]

is basically a peak at \(\omega = 0\), with the width \(\delta \omega = 4\pi / \tau\) and a height of \(f(0) = \tau^2 / 4\). The area under the function \(f(\omega)\) is \(A = \pi \tau / 2\) (see Fig. 2). This means the peak gets higher and narrower as \(\tau\) increases (see Fig. 3).

The height of the peak grows with the square of the time \(\tau\), the area under \(f\) only linearly with \(\tau\). One could thus expect two different behaviors: the square- and the linear regime. At the very beginning, the peak is very broad and therefore much broader than the “band” width \(\delta \epsilon\) divided by \(\hbar\). In this case we expect that the sum grows with the square of \(\tau\), because all terms are near the maximum of the peak (see Fig. 3(b)). We choose some \(\tau_1\) such that the width \(\delta \omega(\tau_1)\) of \(f(\omega)\) has approximately the same value as the “band” width \(\delta \epsilon\) divided by \(\hbar\)

\[
\delta \omega(\tau_1) = \frac{4\pi}{\tau_1} \approx \frac{\delta \epsilon}{\hbar} \quad \Rightarrow \quad \tau_1 = \frac{4\pi \hbar}{\delta \epsilon}. \quad (32)
\]

The terms are distributed over the whole width of the peak and we expect that the sum grows proportional to the area under the peak, thus linearly in \(\tau\) (see Fig. 3(c)). In this case and if, furthermore, the function \(f\) does not change much over many summation steps \(\Delta \omega\), i.e., if

\[
\Delta \omega = \frac{\delta \epsilon}{N_0^2 \hbar} \ll \delta \omega(\tau_1) = \frac{\delta \epsilon}{\hbar} \quad \Rightarrow \quad N_0^2 \gg 1 \quad (33)
\]
the summation averages out the different elements of the $V$-matrix in (28). Therefore the sum may be approximated by the average of the interaction matrix element $\lambda_0^2$ times the integral over $f(\omega)$ according to $\omega$. The average of the interaction matrix element is

$$\lambda_0^2 = \frac{1}{N_1^c N_0^c} \sum_{i=1}^{N_1^c} \sum_{j=1}^{N_0^c} |\langle i | \hat{V} | j \rangle|^2 = \frac{1}{2N_1^c N_0^c} \text{Tr}\{\hat{V}^2\}.$$  

(34)

For (28) we then get

$$|\tilde{U}_1| \approx \lambda_0^2 \int \frac{d\omega}{\Delta \omega} 4f(\omega) = \frac{\lambda_0^2 A}{\Delta \omega} = \frac{2\pi \lambda_0^2 \hbar N_1^c}{\delta \epsilon},$$

(35)

where we have used that the area under $f(\omega)$ is $A = \pi \tau/2$, as mentioned before.

The approximation done so far breaks down later at some time $\tau_2$, when the peak gets too narrow (see Fig. 3(d)), i.e. the width is smaller than the summation displacement $\Delta \omega$

$$\delta \omega(\tau_2) = \frac{4\pi}{\tau_2} = \Delta \omega = \frac{\delta \epsilon}{N_1^c \hbar} \quad \Rightarrow \quad \tau_2 = \frac{4\pi \hbar N_1^c}{\delta \epsilon}.$$  

(36)

Thus (35) is a valid approximation only for $\tau_1 < \tau < \tau_2$, which is the linear regime.

Hence, plugging (35) into (27) yields

$$\text{Tr}_{ex} \left\{ \tilde{U}_1^2 \right\} = \sum_{j=1}^{N_0^c} |\tilde{U}_1| \approx \frac{2\pi \lambda_0^2 \hbar N_1^c N_0^c}{\delta \epsilon} \tau.$$  

(37)

Since this expression is symmetric under exchange of the upper and lower subspace, the corresponding expression for the lower subspace reads

$$\text{Tr}_{gs} \left\{ \tilde{U}_1^2 \right\} = \sum_{i=1}^{N_1^c} |\tilde{U}_1| \approx \frac{2\pi \lambda_0^2 \hbar N_1^c N_0^c}{\delta \epsilon} \tau.$$  

(38)

Inserting (37) and (38) into (26) yields

$$W^{ex}(\tau) = W^{ex}(0) + C\tau N_0^c W^{gs}(0) - C\tau N_1^c W^{ex}(0),$$  

(39)

$$W^{gs}(\tau) = W^{gs}(0) + C\tau N_0^c W^{ex}(0) - C\tau N_1^c W^{gs}(0),$$

where we have abbreviated

$$\frac{2\pi \lambda_0^2}{\delta \epsilon \hbar} := C.$$  

(40)

Equations (39) describe, within the discussed limits, a short time step starting from any initial state, not necessarily an eigenstate of $\hat{H}$. Since they directly connect the probabilities $W^{ex}(0)$, $W^{gs}(0)$ of the initial state with those of the state reached after time $\tau$, we can now iterate these equations under some specific conditions.
7. Conditions on Model Parameters

Before iterating the above equations (39), one should again check the pre-conditions for the short time step equation derived so far. We have only considered terms up to second order, and we can only iterate after a time step of length $\tau_1$. Thus we have to make sure that the considered second order terms are still small compared to 1 after $\tau_1$, to justify the dropping of higher order terms. Therefore we must check that e.g.

$$C\tau N_0^0|_{\tau=\tau_1} = 8\pi^2 \frac{\lambda_0^2}{(\Delta E_0)^2} \frac{1}{N_0} \ll 1,$$  \hspace{1cm} (41)

where we have used (10). In complete analogy we get for the other term of second order

$$C\tau N_1^0|_{\tau=\tau_1} = 8\pi^2 \frac{\lambda_0^2}{(\Delta E_1)^2} \frac{1}{N_1} \ll 1.$$  \hspace{1cm} (42)

If these two conditions are fulfilled the “linear regime” is reached while the truncation to second order is still a valid description, and we can iterate (39) after some time $\tau > \tau_1$. Obviously the linear regime is reached the faster the more levels the environment contains.

However, if we want to use the above scheme (39) we should make sure that we iterate before the linear regime is left again, i.e., before $\tau_2$. Therefore we must consider the second order terms at $\tau_2$ (36) compared to one. Note that $\tau_2$ differs for the two terms of second order, in (36) we only argued for one of the two energy “bands” in the environment. Thus, the case for which iterating (39) is the best description we can possibly get is

$$C\tau N_0^0|_{\tau=\tau_2} = 8\pi^2 \frac{\lambda_0^2}{(\Delta E_0)^2} \geq 1,$$  \hspace{1cm} (43)

$$C\tau N_1^0|_{\tau=\tau_2} = 8\pi^2 \frac{\lambda_0^2}{(\Delta E_1)^2} \geq 1.$$  \hspace{1cm} (44)

8. The Rate Equation

If the above conditions are fulfilled, iterating (39) yields

$$\frac{W^{\text{ex}}((n+1)\tau) - W^{\text{ex}}(n\tau)}{\tau} = C N_0^0 W^{\text{gr}}(n\tau) - C N_1^0 W^{\text{ex}}(n\tau),$$

$$\frac{W^{\text{gr}}((n+1)\tau) - W^{\text{gr}}(n\tau)}{\tau} = C N_1^1 W^{\text{ex}}(n\tau) - C N_0^1 W^{\text{gr}}(n\tau).$$

Or, in the limit of $\tau$ being extremely small

$$\frac{dW^{\text{ex}}}{dt} = C N_0^0 W^{\text{gr}} - C N_1^0 W^{\text{ex}},$$

$$\frac{dW^{\text{gr}}}{dt} = C N_1^1 W^{\text{ex}} - C N_0^1 W^{\text{gr}}.$$  \hspace{1cm} (46)

This evolution equation for the probabilities obviously conserves the overall probability. We have obtained a rate equation for the probabilities to find the system in the upper respectively lower level.

The solutions of the equations (46) describe simple exponential decays, with exactly the same decay rates one would have gotten from Fermi’s Golden Rule. A solution for the considered system being initially entirely in the exited state reads

$$W^{\text{ex}}(t) = \frac{N_0^0}{N_0^0 + N_0^c} + \frac{N_1^c}{N_0^0 + N_1^c} \cdot e^{-C(N_0^0 + N_1^c)t},$$

$$W^{\text{gr}}(t) = \frac{N_1^1}{N_0^0 + N_1^c} \left(1 - e^{-C(N_0^0 + N_1^c)t}\right).$$  \hspace{1cm} (47)

The equilibrium values reached after very long times are

$$W^{\text{ex}}(\infty) = \frac{N_0^c}{N_0^0 + N_0^c}, \quad W^{\text{gr}}(\infty) = \frac{N_1^c}{N_0^0 + N_1^c},$$  \hspace{1cm} (48)

which are exactly the same as the ones derived in [9] for the equilibrium state of a system with an energy exchange coupling to a possibly non-Markovian environment.

9. Numerical Results for the Relaxation Period

To check the validity of the theory developed in the previous Sections, a model of the type depicted in Fig. 1, with a Hamiltonian as described in (11) has been analyzed numerically by directly solving the Schrödinger equation. The interaction matrix $\hat{V}$ has been filled with random Gaussian distributed entries such that

$$\frac{\lambda_0^2}{(\Delta E_0)^2} \approx 1,$$  \hspace{1cm} (49)
to ensure that (41)-(44) are fulfilled. Different container sizes have been analyzed, corresponding to $N_1 = 50, 100, 200, 400, 800$ and $N_0 = \frac{1}{2}N_1$. For all sizes the level spacings $\Delta E_1, \Delta E_0$ have been kept fixed such that for increasing container size the band widths increase.

With those parameter settings the theoretical prediction for $W^\text{gr}(t)$ from (47) is the same for all container sizes. The initial state is always chosen to be a pure product state ($S^g(0) = 0$), with the gas-system in the ground state and the container-system in a random superposition of states from the upper band.

The numerical results are displayed in Fig. 4. The solid line is the prediction from theory. Obviously the theoretical predictions are not accurate for “few-level” container environments. This is due to the fact that the replacement of actual quantities by their Hilbert space average is a valid approximation for high dimensional Hilbert spaces only. Furthermore, for the few-level cases the iteration step times that have to be longer than $\tau_1$ are rather long, because already $\tau_1$ is long. This means that the recursion cannot really be replaced by the differential equation in Sect. 7. This essentially shifts the corresponding curves to later times, compared to the theoretical prediction. All those effects vanish if the container system becomes sufficiently big. The simulation for $N_1 = 800$ is obviously in good agreement with the theoretical prediction.

Fig. 4. Numerical simulation for the relaxation period. The predictions from the rate equation get better with increasing container system, $N_1$.

10. Summary and Conclusion

We considered a two-level system coupled to an environment specified only by two resonant energy bands. We showed that for systems of this type (or rather any bi-partite quantum system) the entropy of the considered system cannot increase without increasing system-environment correlations, if the full system evolution is unitary.

Further more we solved the Schrödinger equation for the full system starting with an initial pure product state. Under some conditions concerning interaction strength, band width and state density of the environment-system we find a merely statistical energy transfer or relaxation process, that may simply be described by some transition rates. This result has been derived on the basis of a theory involving Hilbert space averages and confirmed numerically.

We thus conclude that for statistical decay behavior of exited states in quantum systems neither thermal nor infinite baths are necessary, just as well as the factorizing condition seems neither tenable nor indispensable.

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