On Reduced Time Evolution for Initially Correlated Pure States

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Abstract
A new method to deal with reduced dynamics of open systems by means of the Schrödinger equation is presented. It allows one to consider the reduced time evolution for correlated and uncorrelated initial conditions.
1 Introduction

The study of time evolution of quantum open systems plays an important role in quantum information. The interaction between the system and the reservoir leads to phenomena of dissipation and decoherence [1, 2]. These phenomena can be often modelled through the standard technique of quantum Markov processes in which the density matrix of an open system satisfies the Markovian master equation [3, 4, 5]. However, in the description of complex quantum systems one encounters a complicated non-Markovian behaviour [1, 6–12]. Usually, non-Markovian evolution is studied under the assumption that the initial system-reservoir state is uncorrelated.

The reduced dynamics can be considered in the cases when the state of the total system is mixed or pure. In the latter case, under the assumption of the existence of some symmetries one can solve the Schrödinger equation and deduce the reduced dynamics [13–21]. In the present paper a method to deal with reduced dynamics by means of the Schrödinger equation is presented. It allows one to study the reduced time evolution for correlated and uncorrelated initial conditions, and also makes it possible to consider models beyond the so called rotating wave approximation.

2 A Class of Models

We begin with the description of a class of models of open quantum systems for which the reduced dynamics can be studied in the case when memory effects as well as some initial correlations between the system and the reservoir are taken into account. The method presented here is an extended version of [22].

Let us consider a $d$-level system coupled to the boson field. The associated Hilbert space is $\mathbb{C}^d \otimes \mathcal{F}$ where $\mathcal{F}$ is the bosonic Fock space. Let $|1\rangle, \ldots, |d\rangle$ be a fixed orthonormal base in $\mathbb{C}^d$. The Hamiltonian of the system is assumed to have the form

$$ H = \sum_{i=1}^{d} c_i |i\rangle \langle i| \otimes 1_{\mathcal{F}} + 1_d \otimes H_f + V \quad (2.1) $$

with

$$ H_f = \int d\omega(k) a^*(k)a(k) \quad (2.2) $$

while $V$ is the interaction which is typically chosen in the form

$$ V = \sum_{i,j=1}^{d} |i\rangle \langle j| \otimes a^*(f_{ij}) + \text{h.c.} \quad (2.3) $$

Here $a(k), a^*(k), k \in \mathbb{R}^d$ are annihilation and creation operators on $\mathcal{F}$ and the following notation is used

$$ a(f) = \int d\omega(k) a(k)f(k), \quad (2.4) $$
where
\( f(k) \in L^2(\mathbb{R}^d) \). \hspace{1cm} (2.5)

It is clear that the Schrödinger equation with the above Hamiltonian cannot be solved since one has to deal with the whole Fock space.

In order to restrict the reservoir degrees of freedom the interaction Hamiltonian has to be simplified. Typically, one goes over to the so called V-models \[14\], i.e. one assumes that not all transitions are allowed. More precisely one assumes that
\( f_{ij} \neq 0, \quad i = 2, \ldots, d, \) \hspace{1cm} (2.6)
and all the remaining form-factors vanish. In this case there are invariant sectors in \( \mathbb{C}^d \otimes \mathcal{F} \). In each sector the corresponding Schrödinger equation can be solved. However, there is a different way to simplify the interaction Hamiltonian. Let \( |\Omega\rangle \) be the vacuum state of the boson field, and let
\( P_0 = 1_S \otimes |\Omega\rangle\langle\Omega| \) \hspace{1cm} (2.7)
be the projection operator on \( \mathbb{C}^d \otimes \mathcal{F} \). Following \[22\] let us introduce the approximation \( \tilde{V} \) of \( V \) as follows
\( V \rightarrow \tilde{V} = P_0 V + V P_0 - P_0 V P_0. \) \hspace{1cm} (2.8)

In the case of the interaction \( V \) given in the form \[22,30\], one finds
\( \tilde{V} = \sum_{i,j=1}^{d} |i\rangle\langle j| \otimes a^*(f_{ij})|\Omega\rangle\langle\Omega| + \text{h.c.} \) \hspace{1cm} (2.9)

In this case the only possible transitions in \( \mathcal{F} \) due to \( \tilde{V} \) are
\( |\Omega\rangle \longleftrightarrow a^*(f_{ij})|\Omega\rangle. \) \hspace{1cm} (2.10)

It should be pointed out that the above approximation makes it possible to go beyond the rotating wave approximation.

## 3 Time Evolution and Reduced Dynamics

Let us consider a \( d \)-level system coupled to a bosonic reservoir for which the interaction Hamiltonian is given by \[2.9\]. If the state \( |\phi_t\rangle \) of the coupled system has the form
\[ |\phi_t\rangle = \sum_{i=1}^{d} |i\rangle|c_i(t)|\Omega\rangle + a^*(g_t)|\Omega\rangle, \] \hspace{1cm} (3.1)
the Schrödinger equation is reduced to a closed system of equations for \( c_1(t), \ldots, c_d(t) \) and \( g_t^1(k), \ldots, g_t^d(k) \),
\[ \dot{c}_k(t) = -i\epsilon_k c_k(t) - i \sum_{l=1}^{d} (f_{lk}, g_l^1) \] \hspace{1cm} (3.2)
\[ \dot{g}_t^l = -i(\epsilon_l + \omega(k))g_t^l - i \sum_{n=1}^{d} f_{ln}(k)c_n(t), \] \hspace{1cm} (3.3)
where

\[(f, g) = \int dk \bar{f}(k)g(k)\]  \hspace{1cm} (3.4)

is the scalar product in $L^2(\mathbb{R}^d)$. Moreover, the normalization condition

\[\langle \phi_t | \phi_t \rangle = \langle \phi_0 | \phi_0 \rangle = 1,\]  \hspace{1cm} (3.5)

takes the form

\[\sum_{i=1}^{d} \|c_i(t)\|^2 + (g_{i, i}^t, g_{i, i}^0) = \sum_{i=1}^{d} \|c_i(0)\|^2 + (g_{i, i}^0, g_{i, i}^0) = 1.\]  \hspace{1cm} (3.6)

Equation (3.3) can also be written in the integral form

\[g_{m}^t(k) = e^{-it(\epsilon_m + \omega(k))}g_{m}^0(k) - i\int_{0}^{t} ds e^{-i(t-s)(\epsilon_m + \omega(k))}\sum_{n=0}^{d} f_{mn}(k)c_n(s).\]  \hspace{1cm} (3.7)

Inserting (3.7) into (3.2) one finds a closed system of equations for $c_1(t), \ldots, c_d(t)$,

\[\dot{c}_k(t) = -i\epsilon_k c_k(t) - \int_{0}^{t} ds \sum_{l=1}^{d} M_{kl}(t-s)c_l(s) + G_k(t),\]  \hspace{1cm} (3.8)

where

\[M_{kl}(t) = \sum_{m=1}^{d} \int dk \bar{f}_{mk}f_{ml}e^{-it(\epsilon_m + \omega(k))}\]  \hspace{1cm} (3.9)

and

\[G_k(t) = -i\sum_{m=1}^{d} \int dk \bar{f}_{mk}(k)g_{m}^0(k)e^{-it(\epsilon_m + \omega(k))}.\]  \hspace{1cm} (3.10)

The $M_{kl}(t)$ describe the reservoir correlation functions, while $G_k(t)$ corresponds to correlations between the reservoir and the initial state. Under the assumption that the initial state is given in the form

\[|\phi_0\rangle = \sum_{i=1}^{d} |i\rangle \otimes [c_i(0)|\Omega\rangle + a^*(g_i^0)|\Omega\rangle],\]  \hspace{1cm} (3.11)

the total state $|\phi_t\rangle$ is given by (3.1) in terms of the solution of the equations (3.8), (3.7). It follows from (3.1) that the reduced evolution is given by

\[\text{Tr}_R|\phi_t\rangle \langle \phi_t| = \sum_{i, j=1}^{d} |i\rangle \langle j|[\bar{c}_j(t)c_i(t) + (g_{i, j}^t, g_{j, i}^t)].\]  \hspace{1cm} (3.12)
In order to find explicitly the reduced evolution it is clear that the following correlation functions

\[ a_{mn,pq}(t) = \int dk f_{mn}(k)f_{pq}(k)e^{-i\omega(k)} \]  
\[ b_{mn,p}(t) = \int dk f_{mn}(k)g^p_0(k)e^{-i\omega(k)} \]  
\[ c_{p,q}(t) = \int dk g^p_0(k)g^q_0(k)e^{-i\omega(k)} \]

should be known.

From the above definitions of the correlation functions, it follows that they satisfy the following positivity condition

\[ \sum_{mn} \sum_{pq} a_{mn,pq}(t_\alpha - t_\beta) \bar{x}_{mn}(t_\alpha)x_{pq}(t_\beta) + \sum_{rs} c_{r,s}(t_\alpha - t_\beta) \bar{x}_r(t_\alpha)x_s(t_\beta) + \sum_{mn} \sum_{\beta r} b_{mn,r}(t_\alpha - t_\beta) \bar{x}_{mn}(t_\alpha)x_r(t_\beta) + c.c. \geq 0 \]  

for all sequences of complex numbers \( x_{mn}(t_1), x_{mn}(t_2), x_{mn}(t_3), \ldots \) and \( x_p(t_1), x_p(t_2), \ldots \).

By the Bochner theorem the correlation functions (3.13)–(3.15) can be presented in the form

\[ a_{mn,pq}(t) = \int_{-\infty}^{\infty} d\omega e^{-i\omega t} J_{mn,pq}(\omega), \]  
\[ b_{mn,p}(t) = \int_{-\infty}^{\infty} d\omega e^{-i\omega t} J_{mn,p}(\omega), \]  
\[ c_{pq}(t) = \int_{-\infty}^{\infty} d\omega e^{-i\omega t} J_{pq}(\omega). \]

The matrices \( J_{mn,pq}(\omega) \), \( J_{mn,p}(\omega) \), \( J_{pq}(\omega) \) define the spectral density matrix such that for all sequences \( \{x_{mn}\}, \{x_p\} \) and \( \omega \in \mathbb{R} \) the relation

\[ \sum_{mn} \sum_{pq} J_{mn,pq}(\omega) \bar{x}_{mn}x_{pq} + \sum_{rs} J_{rs}(\omega) \bar{x}_r x_s + \sum_{mnr} J_{mn,r}(\omega) \bar{x}_{mn}x_r + c.c. \geq 0 \]

holds. Thus, choosing the spectral density matrix \( J(\omega) \) one can model the time evolution of the reduced state.

One can distinguish the special type of initial conditions,

\[ |\phi_0\rangle = \left( \sum_{i=1}^{d} |\zeta_i\rangle c_i(0) \right) \otimes |\Omega\rangle, \]
i.e., the simple factorized ones. In this case (3.22) have the form

\[ \dot{c}_k(t) = -i\epsilon_k c_k(t) - \sum_{l=1}^{d} \int_0^t ds M_{kl}(t-s)c_l(s), \quad (3.22) \]

while the relation (3.7) reads

\[ g^m_t(k) = -i \int_0^t ds \sum_{n=0} f_{mn}(k)e^{-i(t-s)(\epsilon_m + \omega(k))}c_n(s). \quad (3.23) \]

Equations (3.22) can be solved using the Laplace transform method, and their solution can be written in the form:

\[ c_k(t) = \sum_{l=1}^{d} L_{kl}(t)c_l(0). \quad (3.24) \]

On the other hand, from (3.23) it follows that

\[ (g^k_t, g^h_t) = \sum_{m,n=1}^{d} R_{km,hn}(t)\bar{c}_m(0)c_n(0). \quad (3.25) \]

It is worth noting that in the case considered the correlation functions (3.13) are needed. Using (3.12), (3.24) and (3.25), one finds that the reduced evolution is given in the form

\[ \text{Tr}_R |\phi_t\rangle \langle \phi_t| = \sum_{jm} \sum_{in} |i\rangle \langle j| S_{jm, in}(t)\bar{c}_m(0)c_n(0), \quad (3.26) \]

where

\[ S_{jm, in}(t) = \bar{L}_{jm}(t)L_{in}(t) + R_{jm, in}(t). \quad (3.27) \]

The relation (3.26) can also be rewritten in the form

\[ \text{Tr}_R |\phi_t\rangle \langle \phi_t| = \sum_{ijm} A_t(|i\rangle \langle j|) c_i(0)\bar{c}_j(0), \quad (3.28) \]

where the relation

\[ A_t(|i\rangle \langle j|) = \sum_{mn} |m\rangle \langle n| S_{nj, mi}(t) \] (3.29)

defines a map

\[ A_t : M_d \longrightarrow M_d, \quad t \geq 0, \quad (3.30) \]

which is completely positive and trace preserving by construction.

The discussion of time evolution under initial conditions different from (3.21) is, in general, very complicated and will be presented on a simple model.
4 Spin-Boson Model beyond the Rotating Wave Approximation

The model is specified by the Hamiltonian

\[ H = \omega \sigma^+ \sigma^- + \int dk \omega(k) a^*(k)a(k) + \sigma^- \otimes a^*(f)|\Omega\rangle\langle\Omega| + \sigma^+ \otimes a^*(h)|\Omega\rangle\langle\Omega| + \text{h.c.} \]

(4.1)
on \mathbb{C}^2 \otimes \mathcal{F} and can be obtained from the spin-boson Hamiltonian containing anti-resonance interaction using the method presented in Sect. 3. The wave function can be chosen in the form

\[ |\phi_t\rangle = (c_0(t)|0\rangle + c_1(t)|1\rangle) \otimes |\Omega\rangle + |0\rangle \otimes a^*(g_0^0)|\Omega\rangle + |1\rangle \otimes a^*(g_1^1)|\Omega\rangle \]

(4.2)
since the interaction in (4.1) allows only the transition between the vacuum state and 1-boson states. The Schrödinger equation is equivalent to the following set of equations for \( c_0(t), c_1(t) \) and \( g_0^0(t), g_1^1(t) \):

\[ \dot{c}_0 = -(h, g_1^1), \]

(4.3)
\[ \dot{c}_1 = -i\omega c_1(t) - i(f, g_0^0), \]

(4.4)
\[ \dot{g}_0^0(k) = -i\omega(k)g_0^0(k) - if(k)c_1(t), \]

(4.5)
\[ \dot{g}_1^1(k) = -i(\omega + \omega(k))g_1^1(k) + h(k)c_0(t). \]

(4.6)
Equations (4.4) and (4.5) are the same as in the case of spin-boson model in the rotating wave approximation. On the other hand (4.3), (4.6) describe the effect of anti-resonance interaction. It follows from (4.3) – (4.6) that our system has two constants of motion:

\[ |c_0(t)|^2 + (g_1^1, g_1^1) = |c_0(0)|^2 + (g_0^0, g_0^0) = p_0 \geq 0 \]

(4.7)
and

\[ |c_1(t)|^2 + (g_0^0, g_0^0) = |c_1(0)|^2 + (g_0^0, g_0^0) = p_1 \geq 0 \]

(4.8)
Moreover, the normalization condition

\[ \langle \phi_t | \phi_t \rangle = \langle \phi_0 | \phi_0 \rangle = 1, \]

(4.9)
takes the form

\[ p_0 + p_1 = 1. \]

(4.10)
The reduced state \( \text{Tr}_R(\phi_t | \phi_t) \) can be written as follows

\[ \rho(t) = \text{Tr}_R(\phi_t | \phi_t) = \sum_{i,j=0}^{1} \langle i|j \rangle \rho_{ij}(t), \]

(4.11)
where

\[ \rho_{00}(t) = |c_0(t)|^2 + (g_0^0, g_0^0) \]

(4.12)
\[ \rho_{11}(t) = |c_1(t)|^2 + (g_1^1, g_1^1) \]

(4.13)
\[ \rho_{01}(t) = \rho_{10}(t) = c_0(t)c_1(t) + (g_0^1, g_1^0). \]

(4.14)
Using (4.7) and (4.8) the diagonal elements of $\rho(t)$ can be written in the form

$$\rho_{00}(t) = |c_0(t)|^2 + |c_1(0)|^2 - |c_1(t)|^2 + (g_0^0, g_0^0) \quad (4.15)$$
$$\rho_{11}(t) = 1 - \rho_{00}(t). \quad (4.16)$$

It should be pointed out that the equations (4.3), (4.6) and (4.4), (4.5) are independent. However, there exists coupling in terms of correlation functions which are needed to calculate the reduced evolution. Eliminating $g_0^0(k)$ and $g_1^1(k)$ from (4.5) and (4.6) the following equations for $c_0(t)$ and $c_1(t)$ can be derived

$$\dot{c}_0(t) = \int_0^t ds \ m_0(t-s)c_0(s) + n_0(t), \quad (4.17)$$
$$\dot{c}_1(t) = -i\omega c_1(t) - \int_0^t ds \ m_1(t-s)c_1(s) + n_1(t), \quad (4.18)$$

where

$$m_0(t) = \int dk |h(k)|^2 e^{-it(\omega + \omega(k))}, \quad (4.19)$$
$$m_1(t) = \int dk |f(k)|^2 e^{-it\omega(k)} \quad (4.20)$$

and

$$n_0(t) = -i \int dk \ h(k)g_0^1(k)e^{-it(\omega + \omega(k))}, \quad (4.21)$$
$$n_1(t) = -i \int dk \ f(k)g_0^0(k)e^{-it\omega(k)}. \quad (4.22)$$

In order to find out an explicit form of $\rho(t)$ a detailed knowledge of all the correlation functions is required. However, general properties of $\rho_{00}(t)$ and $\rho_{11}(t)$ can be deduced in the following manner. Suppose that $A_0(t)c_0(0)$ and $A_1(t)c_1(0)$ are general solutions of homogeneous equations (4.17) and (4.18), respectively. Then one has

$$c_\alpha(t) = A_\alpha(t)c_\alpha(0) + \int_0^t ds \ A_\alpha(t-s)n_\alpha(s) \quad (4.23)$$

with $\alpha = 0, 1$ and

$$\rho_{00}(t) = |c_0(t)|^2 + |c_1(0)|^2 - |c_1(t)|^2 + (g_0^0, g_0^0). \quad (4.24)$$

It follows from (4.23) that the time dependence of $\rho_{00}(t)$ is related to the initial conditions. Moreover, the asymptotic behaviour of $\rho_{00}(t)$ can be easily found as

$$\lim_{t \to \infty} \rho_{00}(t) = |c_1(0)|^2 + (g_0^0, g_0^0) \quad (4.25)$$
since, typically, one has
\[
\lim_{t \to \infty} c_\alpha(t) = 0, \quad \alpha = 0, 1.
\] (4.26)

The formula (4.25) shows that the asymptotic state is determined by the initial conditions, i.e., the equilibrium state does not exist. In the case \( g_0^0(k) = g_0^1(k) = 0 \) the time evolution is given in terms of a completely positive and trace preserving but not relaxing map.

The spin-boson model is recovered if one puts \( h(k) = 0 = g_0^0(k) = g_1^1(t) \). In this case we have
\[
|c_0(t)|^2 = |c_1(0)|^2
\] (4.27)
and, using the normalization condition (4.8) one finds
\[
\rho_{00}(t) = 1 - |c_1(t)|^2
\] (4.28)
\[
\rho_{11}(t) = |c_1(t)|^2.
\] (4.29)

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