Exact solution of the Schrödinger equation with the spin-boson Hamiltonian

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Abstract
We address the problem of obtaining the exact reduced dynamics of the spin-half (qubit) immersed within the bosonic bath (environment). An exact solution of the Schrödinger equation with the paradigmatic spin-boson Hamiltonian is obtained. We believe that this result is a major step ahead and may ultimately contribute to the complete resolution of the problem in question. We also construct the constant of motion for the spin-boson system. In contrast to the standard techniques available within the framework of the open quantum systems theory, our analysis is based on the theory of block operator matrices.

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1. Introduction

The Hamiltonian of the paradigmatic spin-boson (SB) model is specified as [1–4]

$$ H_{SB} = H_S \otimes I_B + I_S \otimes H_B + H_{int}, $$

where

$$ H_S = (\beta \sigma_z + \alpha \sigma_x) \quad \text{and} \quad H_B = \int_0^\infty d\omega \, h(\omega) \, a^\dagger(\omega) a(\omega), $$

are the Hamiltonian of the spin-half (qubit) and the bosonic field (environment), respectively. The interaction between the systems has the following form:

$$ H_{int} = \sigma_z \otimes \int_0^\infty d\omega (g(\omega)^* a(\omega) + g(\omega) a^\dagger(\omega)) \equiv \sigma_z \otimes V. $$

$I_S$ and $I_B$ are the identity operators in corresponding Hilbert spaces of the qubit and the environment, respectively.

In the above description, $\sigma_z$ and $\sigma_x$ are the standard Pauli matrices. The bosonic creation $a^\dagger(\omega)$ and annihilation $a(\omega)$ operators obey the canonical commutation relation: $[a(\omega), a^\dagger(\eta)] = \delta(\omega - \eta) I_B$, for $\omega, \eta \in [0, \infty)$. The functions $h, g \in L^2[0, \infty]$ model
the energy of the free bosons and the coupling the bosons with the qubit, respectively. The constants $\alpha$ and $\beta$ are assumed to be real and non-negative numbers. Furthermore, $\beta$ represents the energy gap between the eigenstates $|0\rangle$ and $|1\rangle$ of $\sigma_z$, while $\alpha$ is responsible for the tunneling between these states. The Hamiltonian (1) acts on the total Hilbert space $\mathcal{H}_{\text{tot}} = \mathcal{C}^2 \otimes \mathcal{F}_B$, where $\mathcal{F}_B := \mathcal{F}(L^2[0, \infty])$ is the bosonic Fock space [5].

It is worth mentioning that more often we encounter situations in which there is a countable number (finite, in particular) of bosons (see e.g., [6–9]). In such cases we define the SB model via the following Hamiltonian:

$$H_{\text{SB}} = (\beta \sigma_z + \alpha \sigma_x) \otimes \mathbb{I}_B + \mathbb{I}_S \otimes \sum_k h_k a_k^\dagger a_k + \sigma_z \otimes \sum_k (g_k^* a_k + g_k a_k^\dagger), \quad (4)$$

where the creation and annihilation operators $a_k^\dagger, a_k$ satisfy $[a_k, a_l^\dagger] = \delta_{kl}$. Formally, it is possible to obtain (4) from (1) by setting

$$x(\omega) = \sum_k x_k \delta(\omega - \omega_k), \quad (5)$$

Therefore, we can treat both cases simultaneously. Although generalizations of the SB model (e.g., asymmetric coupling [10]) are also under intensive investigation, we will not focus on them in this paper.

The problem of a small quantum system coupled to the external degrees of freedom plays an important role in various fields of modern quantum physics. The SB model provides a simple mathematical description of such coupling in the case of two-level quantum systems. For instance, an interaction between two-level atoms and the electromagnetic radiation can be modeled via the SB Hamiltonian [11]. For this reason the SB model is of great importance to the modern quantum optics. There are various physical problems (e.g., decoherence [12–15], geometric phase [16]) related to the properties of the model in question, which have already been addressed and intensively discussed. Nonetheless, an exact solution of the Schrödinger equation,

$$i\partial_t |\Psi_t\rangle = H_{\text{SB}} |\Psi_t\rangle \quad \text{with} \quad |\Psi_0\rangle \equiv |\Psi\rangle, \quad (6)$$

is still missing for both $\alpha \neq 0$ and $\beta \neq 0$. Several approximation methods [17] have been developed in the past 50 years to manage this problem. Models obtained from the SB Hamiltonian under mentioned approximations are well-established and in most cases they are exactly solvable. The famous Jaynes–Cummings model [18] can serve as an example. Formally, one can always express the solution of (6) as $|\Psi_t\rangle = U_t |\Psi\rangle$, where $U_t := \exp(-iH_{\text{SB}} t)$ is the time evolution operator (Stone theorem [19]). Needless to say, such a form of the solution is useless for practical purposes.

There is at least one important reason for which a manageable form of the time evolution operator $U_t$ is worth seeking. Namely, it allows us to construct the exact reduced time evolution of the spin immersed within the bosonic bath, the so-called reduced dynamics [20]:

$$\rho_t = \text{Tr}_B \left( U_t \rho_0 \otimes \omega_B U_t^\dagger \right). \quad (7)$$

Above, the state $\omega_B$ is an initial state of the bosonic bath. $\text{Tr}_B$ denotes the partial trace, i.e. $\text{Tr}_B (M \otimes X) = \text{MTr}X$, where Tr refers to the usual trace on $\mathcal{F}_B$. For the sake of simplicity, we have assumed that the initial state of the composite system $\rho_0$ is the tensor product of the states $\rho_0$ and $\omega_B$. In other words, no initial correlations between the systems are present [21–24].

In general, formula (7) is far less useful than its theoretical simplicity might indicate. Indeed, to trace out the state $U_t \rho_0 U_t^\dagger$ over the bosonic degrees of freedom, one needs to (i)
calculate $U_t$ and (ii) apply the result to the initial state $\rho_{\text{int}}$. Herein, we will cover the first step and investigate the ability to accomplish the second one.

In order to write the time evolution operator $U_t$ in a computationally accessible form, the diagonalization of its generator $H_{SB}$ or an appropriate factorization [25] is required. It can be found (see e.g., [26–28]) that the problem of diagonalization on the Hilbert space $\mathbb{C}^2 \otimes \mathcal{F}_B$ can be mapped to the problem of resolving the Riccati equation [29]. This new approach was recently successfully applied to the time-dependent spin-spins model [30]. As a result, the exact reduced dynamics of the qubit in contact with a spin environment and in the presence of a precessing magnetic field has been obtained. It is interesting, therefore, to apply this approach to the SB model as well. This paper is devoted to accomplishing this purpose. Although, an explicit form of the Riccati equation has already been derived [31], the solution has not yet been provided. In this paper, we derive an exact solution of this equation assuming $\beta = 0$.

2. The block operator matrix representation and the Riccati equation

We begin by reviewing some basic facts concerning a connection between the theory of block operator matrices [32] and the SB model. First, the Hamiltonian (1) admits the block operator matrix representation [31, 33]:

$$H_{SB} = \begin{bmatrix} H_B + V + \beta & \alpha \\ \alpha & H_B - V - \beta \end{bmatrix} \equiv \begin{bmatrix} H_+ & \alpha \\ \alpha & H_- \end{bmatrix},$$

(8)

with respect to the direct sum decomposition $H_{\text{tot}} = \mathcal{F}_B \oplus \mathcal{F}_B$ of $H_{\text{tot}}$. The entries $\alpha$ and $\beta$ of the operator matrix (8) are understood as $\alpha I_B$ and $\beta I_B$, respectively. Henceforward, we use the same abbreviation for any complex number.

The Riccati operator equation associated with matrix (8) reads [31]

$$\alpha X^2 + XH_+ - H_-X - \alpha = 0,$$

(9)

where $X$ is an unknown operator, acting on $\mathcal{F}_B$, which needs to be determined. The solution of this equation, if it exists, can be used to diagonalize the Hamiltonian (8). To be more specific, if $X$ solves (9) the following equality holds true:

$$S^{-1}H_{SB}S = \begin{bmatrix} H_+ + \alpha X & 0 \\ 0 & H_- - \alpha X \end{bmatrix}, \quad \text{where} \quad S = \begin{bmatrix} 1 & -X^\dagger \\ X & 1 \end{bmatrix}. $$

(10)

By means of this decomposition we can write $U_t$ in an explicit matrix form:

$$U_t = S \text{diag}[e^{-i(H_+ + \alpha X)t}, e^{-i(H_- - \alpha X)\dagger t}]S^{-1}. $$

(11)

Note that the last formula reduces the problem of finding the solution of the Schrödinger equation (6) to the problem of resolving the Riccati equation (9). It is well established that the reduced dynamics (7) can easily be obtained when $\alpha = 0$ [5]. In this case no additional assumptions on $\beta$ are needed, which should not be surprising since the matrix (8) is already in a diagonal form ($X = 0$). Moreover, if $\alpha = 0$ the qubit does not exchange the energy with the bosonic field because $[H_B \otimes I_B, H_{SB}] = 0$. Therefore, the only exactly solvable case, which is known at the present time, represents a rather extreme physical situation.

In the next section, we will derive an exact solution of the RE (9) assuming $\beta = 0$; nevertheless, we do not impose any restrictions on $\alpha$. This is exactly the opposite situation to the one we have discussed above. At this point, the natural question can be addressed: what about the case when both $\alpha$ and $\beta$ are not equal to zero? Unfortunately, the answer is still to be found. In fact, usually the SB model is defined only for $\beta = 0$. At first, it might seem that the complexity of the problem is the same both for $\beta = 0$ and $\beta \neq 0$. Although this is indeed true when $\alpha = 0$, no argument proving this conjecture for $\alpha \neq 0$ has been given so far. We will return to this matter at the end of the next section.
3. Solution of the Riccati equation

3.1. Single boson case

To understand the idea of our approach better let us first consider the case where there is only one boson in the bath [34, 35]. Then, the Hamiltonian of the SB model can be written by using the block operator matrix nomenclature as (β = 0)

\[
H_{SB} = \begin{bmatrix} H_\uparrow & \alpha \\ \alpha & H_\downarrow \end{bmatrix} \quad \text{with} \quad H_\downarrow = \omega a^\dagger a \pm (g^* a + ga^\dagger).
\]

The operators \(H_\downarrow\) can be expressed in a more compact form, that is

\[
H_\downarrow = \omega D_f a^\dagger a D_{-f} - E \quad \text{and} \quad H_\uparrow = \omega D_{-f} a^\dagger a D_f - E,
\]

where \(f = g/\omega\) and \(E = |g|^2/\omega\). The displacement operator \(D_f := \exp(f^*a - fa^\dagger)\) has the following, easy to prove, properties:

(i) \(D_{-f} = D_f^\dagger\),
(ii) \(D_f D_{-f} = I_B\)
(iii) \(D_f D_{-f} = e^{i(f^*a - fa^\dagger)}D_{-f}e^{fg}\).

3 stands for the imaginary part of the complex number \(fg^*\). Relations (13) can be proven by using equality \(D_f a D_{-f} = a - f\), which follows from the Baker–Campbell–Hausdorff formula [36, 37]. For the sake of simplicity and without essential loss of generality we rescale the Hamiltonian (12) so that \(H_{SB} \rightarrow H_{SB} + E\). This is nothing but a rescaling of the reference point of the total.

After this procedure the Hamiltonian (12) takes the form

\[
H_{SB} = \begin{bmatrix} \omega D_f a^\dagger a D_{-f} & \alpha \\ \alpha & \omega D_{-f} a^\dagger a D_f \end{bmatrix},
\]

while the corresponding Riccati equation reads

\[
\alpha X^2 + X \left(\omega D_f a^\dagger a D_{-f} - \omega D_{-f} a^\dagger a D_f \right) X - \alpha = 0.
\]

To solve this equation, let us first define an operator \(P_\varphi\) in a way that

\[
P_\varphi := \exp(i\varphi a^\dagger a), \quad \varphi \in [0, 2\pi).
\]

It is not difficult to see that

(i) \(P_\varphi = P_\varphi^\dagger\),
(ii) \(P_\pi P_\varphi = I_B\) and
(iii) \(P_\varphi P_\varphi = P_{\varphi^*\varphi}\).

Moreover, from the Baker–Campbell–Hausdorff formula we also have \(P_\varphi a P_{-\varphi} = e^{-i\varphi}a\), which ultimately leads to

\[
P_\pi D_f P_{-\varphi} = D_{\varphi^*f}.
\]

In what follows, we will prove that \(P_\pi\) solves the Riccati equation (16). First, let us note that \(P_\pi\) is a function of the number operator \(a^\dagger a\), thus \([P_\pi, a^\dagger a] = 0\). In view of (19) we obtain \(P_\pi D_f P_{-\varphi} = D_{\varphi^*f}\), hence,

\[
P_\pi (D_f a^\dagger a D_{-f}) = (D_{-f} a^\dagger a D_f) P_\pi.
\]

By writing \(P_\pi\) in terms of the eigenstates \(|n\rangle\) of \(a^\dagger a\) we obtain

\[
P_\pi = \sum_{n \in \mathbb{N}} e^{i\pi n}|n\rangle \langle n| = \sum_{n \in \mathbb{N}} (-1)^n |n\rangle \langle n|,
\]

where we used the well-known mathematical fact that \(a^\dagger a|n\rangle = n|n\rangle\), for \(n \in \mathbb{N}\). Finally, from (21) we conclude that \(P_\pi\) is an involution, i.e. \(P_\pi^2 = I_B\), which together with (20) leads to

\[
\alpha P_\pi^2 + P_\pi (\omega D_f a^\dagger a D_{-f}) - (\omega D_{-f} a^\dagger a D_f) P_\pi - \alpha = 0.
\]

\[\text{J. Phys. A: Math. Theor. 44 (2011) 195301} \quad \text{B Gardas}\]
Note, $P_\pi$ transforms the creation $a^\dagger$ and annihilation $a$ operators into $-a^\dagger$ and $-a$, respectively. In other words, $P_\pi$ can be interpreted as the bosonic parity operator [38]. Moreover, $P_\pi$ does not depend on the parameter $\alpha$; in particular, $P_\pi$ remains a nontrivial ($X \neq 0$) solution of the Riccati equation (16) even when $\alpha = 0$ (Sylvester equation).

Now, by means of the parity operator $P_\pi$, we can derive an accessible form of the time evolution operator $U_t$. According to (10) and (11) we have

\[
U_t = \frac{1}{2} \begin{bmatrix}
U_+(t) & V_+(t)P_\pi \\
V_+(t)P_\pi & U_-(t)
\end{bmatrix},
\]

where the quantities $U_\pm(t)$ and $V_\pm(t)$ read as follows

\[
U_\pm(t) = e^{-i(H_\pm + \alpha P_\pi)t} + e^{-i(H_\pm - \alpha P_\pi)t},
\]

\[
V_\pm(t) = e^{-i(H_\pm + \alpha P_\pi)t} - e^{-i(H_\pm - \alpha P_\pi)t}.
\]

For $\alpha = 0$ the formula (23) simplifies to the well-known result [5], which can be obtained independently, without solving the Riccati equation.

It is instructive to see how the bosonic parity operator $P_\pi$ can also be used to construct the constant of motion for the SB model. For this purpose let us take $J_\pi := \sigma_x \otimes P_\pi$, then $[J_\pi, H_{SB}] = 0$, thus from the Heisenberg equations of motion follows $J_\pi = 0$, which means that $J_\pi$ does not vary with time. Since $P_\pi$ is an involution, i.e., $P_\pi^2 = I_B$ thus $J_\pi$ is an involution as well. Therefore, $J_\pi$ can be seen as the parity operator of the total system. In conclusion, the total parity is conserved when $\beta = 0$.

For $\beta \neq 0$ the parity symmetry of the total system is broken and the Riccati equation (16) cannot be solved by applying a similar method to the one we have used above in the case of $\beta = 0$. From mathematical point of view, the problem arises because the diagonal entries $H_B \pm \beta$ are no longer related by a unitary transformation. Indeed, if the converse was true, there would then exist an unitary operator $W$ such that $W^\dagger (H_B + V + \beta) W = H_B - V - \beta$. Thereby, the spectra $\sigma(H_B \pm V \pm \beta) = \sigma(H_B \pm V) \cup \{\pm \beta\}$ would be the same, which clearly is impossible unless $\beta = 0$. As a result, for $\alpha \neq 0$ one can expect that the mathematical complexity of the SB model is different within the regimes $\beta = 0$ and $\beta \neq 0$.

3.2. Generalization

The results of the preceding subsection can be generalized to the case where there is more that one boson in the bath. In order to achieve this objective one needs to redefine the displacement operator $D_f$ in the following way:

\[
D_f \rightarrow \exp(A - A^\dagger), \quad \text{where} \quad A = \sum_k \frac{g_k^*}{\omega_k} a_k.
\]

Then, the solution of the Riccati equation reads

\[
P = \exp \left(i \tau \sum_k a_k^* a_k \right) = \bigotimes_k P_{\pi,k}, \quad \text{where} \quad P_{\pi,k} = \exp \left(i \pi a_k^* a_k \right).
\]

4. Remarks and summary

In this paper, we have solved the Riccati operator equation associated with the Hamiltonian of the paradigmatic SB model. Next, in terms of the solution we have derived an explicit matrix form of the time evolution operator of the total system. This, in particular, allows us to solve the Schrödinger equation (6). We wish to emphasize that in order to obtain the reduced dynamics (7) one more step is required. Namely, the terms such as

\[
\text{Tr}(e^{-i[H_x \pm \alpha P_\pi]t} \rho_B e^{i[H_x \pm \alpha P_\pi]t})
\]

(27)
need to be determined. Of course, one can always evaluate the quantities given above by using e.g., perturbation theory. However, the true challenge is to establish this goal without approximations. It seems that the simplest way to do so is to solve the eigenvalue problem \((H_\pm \pm \alpha P_\pi)|\psi\rangle = \lambda|\psi\rangle\). The ability to solve this eigenproblem separates us from deriving the exact reduced dynamics of the qubit immersed within the bosonic bath. We stress that for \(\alpha \neq 0\) the problem is nontrivial since the qubit exchange the energy with its environment. Moreover, an impact on the mathematical complexity of the model has not only a transfer of the energy between the systems, but also the energy split between the states \([0]\), \([1]\).

Interestingly, the Riccati equation is a second-order operator equation; thus one can expect that its solution involves a square root. In particular, nothing indicates that the solution should be linear as it is in our case. Therefore, we not only solved the Riccati equation (9) but also linearized the solution. At this point, a worthwhile question can be posed: is it a coincidence that the linear operator happens to solve a nonlinear equation? Perhaps, it is a manifestation of some additional structure in the model. Historically, a similar situation took place when Dirac solved the problem with a negative probability by introducing his famous equation [39]. By linearizing the Hamiltonian of the relativistic electron, Dirac not only predicted the existence of antiparticles, but also explained the origin of the additional degree of freedom of the electron.

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References

[1] Fannes M, Nachtergaele B and Verbeure A 1988 The equilibrium states of the spin-boson model Commun. Math. Phys. 114 537–48
[2] Fannes M, Nachtergaele B and Verbeure A 1988 Tunneling in the equilibrium state of a spin-boson model J. Phys. A: Math. Gen. 21 1759
[3] Spohn H 1989 Ground state(s) of the spin-boson hamiltonian Commun. Math. Phys. 123 277–304
[4] Honegger R 1991 On the dynamics and the temperature states of the spin-boson model Phys. Rev. A 21 351–9
[5] Alicki R 2004 Pure decoherence in quantum system Open Sys. Inf. Dyn. 11 53–61
[6] Leggett A J et al 1987 Dynamics of the dissipative two-state system Rev. Mod. Phys. 59 1–85
[7] Allahverdyan A E, Graciá R S and Nieuwenhuizen Th M 2005 Work extraction in the spin-boson model Phys. Rev. E 71 046106
[8] Kehrein S K and Mielke A 1996 On the spin-boson model with a sub-ohmic bath Phys. Lett. A 219 313–8
[9] Salkola M I et al 1996 Coupled spin-boson systems far from equilibrium Phys. Rev. B 54 R12645–8
[10] Dajka J, Mierzejewski M and Łuczka J 2009 Fidelity of asymmetric dephasing channels Phys. Rev. A 79 012104
[11] Puri R 2001 Mathematical Methods of Quantum Optics (Berlin: Springer)
[12] Zurek W H 2003 Decoherence, einselection, and the quantum origins of the classical Rev. Mod. Phys. 75 715–75
[13] Dajka J et al 2010 Dephasing of qubits by the Schrödinger cat Physica E 42 374–7
[14] Dajka J and Łuczka J 2008 Origination and survival of qudit–qudit entanglement in open systems Phys. Rev. A 77 062303
[15] Dajka J, Mierzejewski M and Łuczka J 2008 Non-Markovian entanglement evolution of two uncoupled qubits Phys. Rev. A 77 042316
[16] Dajka J, Łuczka J and Hänggi P 2011 Geometric phase as a determinant of a qubit–environment coupling Quantum Inf. Process. 10 85–96
[17] Davies E B 1976 Quantum Theory of Open Systems (London: Academic)
[18] Romanelli A 2009 Generalized Jaynes–Cummings model as a quantum search algorithm Phys. Rev. A 80 014302
[19] Reed M and Simon B 1980 Method of Modern Mathematical Physics (London: Academic)
[20] Alicki R and Lendi K 2007 *Quantum Dynamical Semigroups and Applications* 2nd edn (Springer Lecture Notes in Physics vol 717) (Berlin: Springer)

[21] Štelmachović P and Bužek V 2001 Dynamics of open quantum systems initially entangled with environment: beyond the Kraus representation *Phys. Rev. A* **64** 062106

[22] Štelmachović P and Bužek V 2003 Dynamics of open quantum systems initially entangled with environment: beyond the Kraus representation *Phys. Rev. A* **67** 022902 (Erratum)

[23] Hayashi H, Kimura G and Ota Y 2003 Kraus representation in the presence of initial correlations *Phys. Rev. A* **67** 062109

[24] Dajka J and Łuczka J 2010 Distance growth of quantum states due to initial system-environment correlations *Phys. Rev. A* **82** 012341

[25] García Quijas P C and Arévalo Aguilar L M 2007 Factorizing the time evolution operator *Phys. Scr.* **75** 185–94

[26] Gardas B 2009 Almost pure decoherence *Master’s Thesis* University of Silesia, Poland

[27] Adamjan V, Langer H and Tretter C 2001 Existence and uniqueness of contractive solutions of some Riccati equations *J. Funct. Anal.* **179** 448–73

[28] Gardas B 2011 Riccati equation and the problem of decoherence II: Symmetry and the solution of the Riccati equation *J. Math. Phys.* at press (arXiv:1006.1931v1)

[29] Kostrykin V, Makarov K and Motovilov A 2003 Existence and uniqueness of solutions to the operator Riccati equation. A geometric approach *Contemp. Math.* **327** 181–98

[30] Gardas B 2010 Exact reduced dynamics for a qubit in a precessing magnetic field and in contact with a heat bath *Phys. Rev. A* **82** 042115

[31] Gardas B 2010 Riccati equation and the problem of decoherence *J. Math. Phys.* **51** 062103

[32] Tretter C 2008 *Spectral Theory of Block Operator Matrices and Applications* (London: Imperial College Press)

[33] Langer H and Tretter C 1998 Spectral decomposition of some non-selfadjoint block operator matrix *J. Operator Theory* **39** 339–59

[34] Jaynes E T and Cummings F W 1963 Generalized Jaynes–Cummings model as a quantum search algorithm *Proc. IEEE* **51** 89–109

[35] Cummings F W 1965 Stimulated emission of radiation in a single mode *Phys. Rev. A* **140** A1051–6

[36] Galindo A and Pascual P 1990 *Quantum Mechanics I* (Berlin: Springer)

[37] Ebrahimi-Fard K, Guo L and Manchon D 2006 Birkhoff-type decompositions and the Baker–Campbell–Hausdorff recursion *Commun. Math. Phys.* **267** 821–45

[38] Bender C M, Meisinger P N and Wang Q 2003 All Hermitian Hamiltonians have parity *J. Phys. A: Math. Gen.* **36** 1029

[39] Thuller B 1992 *The Dirac Equation* (New York: Springer)