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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]

$$\mathbf{H}_{\mathrm{SB}} = \mathrm{H}_{\mathrm{S}} \otimes \mathbb{I}_{\mathrm{B}} + \mathbb{I}_{\mathrm{S}} \otimes \mathrm{H}_{\mathrm{B}} + \mathbf{H}_{\mathrm{int}}, \tag{1}$$

where

$$\mathrm{H}_{\mathrm{S}} = (\beta\sigma_z + \alpha\sigma_x) \quad \text{and} \quad \mathrm{H}_{\mathrm{B}} = \int_0^\infty \mathrm{d}\omega\, h(\omega)\, a^\dagger(\omega)a(\omega), \tag{2}$$

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

$$\mathbf{H}_{\mathrm{int}} = \sigma_z \otimes \int_0^\infty \mathrm{d}\omega (g(\omega)^* a(\omega) + g(\omega)a^\dagger(\omega)) \equiv \sigma_z \otimes \mathrm{V}. \tag{3}$$

$\mathbb{I}_{\mathrm{S}}$ and $\mathbb{I}_{\mathrm{B}}$ are the identity operators in corresponding Hilbert spaces of the qubit and the environment, respectively.

In the above description, σ_z and σ_x are the standard Pauli matrices. The bosonic creation $a^\dagger(\omega)$ and annihilation $a(\omega)$ operators obey the canonical commutation relation: $[a(\omega), a^\dagger(\eta)] = \delta(\omega - \eta)\mathbb{I}_{\mathrm{B}}$, 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 α and β are assumed to be real and non-negative numbers. Furthermore, β represents the energy gap between the eigenstates $|0\rangle$ and $|1\rangle$ of σ_z, while α is responsible for the tunneling between these states. The Hamiltonian (1) acts on the total Hilbert space $\mathcal{H}_{\text{tot}} = \mathbb{C}^2 \otimes \mathcal{F}_{\text{B}}$, where $\mathcal{F}_{\text{B}} := \mathcal{F}(L^2[0, \infty])$ 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:

$$\mathbf{H}_{\text{SB}} = (\beta\sigma_z + \alpha\sigma_x) \otimes \mathbb{I}_{\text{B}} + \mathbb{I}_{\text{S}} \otimes \sum_k h_k a_k^\dagger a_k + \sigma_z \otimes \sum_k (g_k^* a_k + g_k a^\dagger), \tag{4}$$

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

$$x(\omega) = \sum_k x_k \delta(\omega - \omega_k), \quad \text{where} \quad x = h, g. \tag{5}$$

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,

$$\mathrm{i}\partial_t|\Psi_t\rangle = \mathbf{H}_{\text{SB}}|\Psi_t\rangle \quad \text{with} \quad |\Psi_0\rangle \equiv |\Psi\rangle, \tag{6}$$

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 $|\Psi_t\rangle = \mathbf{U}_t|\Psi\rangle$, where $\mathbf{U}_t := \exp(-\mathrm{i}\mathbf{H}_{\text{SB}}t)$ 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 $\mathbf{U}_t$ 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]:

$$\rho_t = \text{Tr}_{\text{B}}\big(\mathbf{U}_t \rho_0 \otimes \omega_{\text{B}} \mathbf{U}_t^\dagger\big). \tag{7}$$

Above, the state ω_{B} is an initial state of the bosonic bath. Tr_{B} denotes the partial trace, i.e. $\text{Tr}_{\text{B}}(\text{M} \otimes X) = \text{M}\text{Tr}X$, 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 ρ_{int} is the tensor product of the states ρ_0 and ω_{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 $\mathbf{U}_t \rho_{\text{int}} \mathbf{U}_t^\dagger$ over the bosonic degrees of freedom, one needs to (i) calculate $\mathbf{U}_t$ and (ii) apply the result to the initial state ρ_{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 $\mathbf{U}_t$ in a computationally accessible form, the diagonalization of its generator $\mathbf{H}_{\mathrm{SB}}$ 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 $\mathbb{C}^2 \otimes \mathcal{F}_{\mathrm{B}}$ 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]:

$$\mathbf{H}_{\mathrm{SB}} = \begin{bmatrix} \mathrm{H_B} + \mathrm{V} + \beta & \alpha \\ \alpha & \mathrm{H_B} - \mathrm{V} - \beta \end{bmatrix} \equiv \begin{bmatrix} \mathrm{H}_+ & \alpha \\ \alpha & \mathrm{H}_- \end{bmatrix}, \tag{8}$$

with respect to the direct sum decomposition $\mathcal{H}_{\mathrm{tot}} = \mathcal{F}_{\mathrm{B}} \oplus \mathcal{F}_{\mathrm{B}}$ of $\mathcal{H}_{\mathrm{tot}}$. The entries α and β of the operator matrix (8) are understood as $\alpha\mathbb{I}_{\mathrm{B}}$ and $\beta\mathbb{I}_{\mathrm{B}}$, respectively. Henceforward, we use the same abbreviation for any complex number.

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

$$\alpha X^2 + X\mathrm{H}_+ - \mathrm{H}_- X - \alpha = 0, \tag{9}$$

where X is an unknown operator, acting on $\mathcal{F}_{\mathrm{B}}$, 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:

$$\mathbf{S}^{-1}\mathbf{H}_{\mathrm{SB}}\mathbf{S} = \begin{bmatrix} \mathrm{H}_+ + \alpha X & 0 \\ 0 & \mathrm{H}_- - \alpha X^\dagger \end{bmatrix}, \quad \text{where} \quad \mathbf{S} = \begin{bmatrix} 1 & -X^\dagger \\ X & 1 \end{bmatrix}. \tag{10}$$

By means of this decomposition we can write $\mathbf{U}_t$ in an explicit matrix form:

$$\mathbf{U}_t = \mathbf{S}\,\mathrm{diag}[\mathrm{e}^{-\mathrm{i}(\mathrm{H}_+ + \alpha X)t}, \mathrm{e}^{-\mathrm{i}(\mathrm{H}_- - \alpha X^\dagger)t}]\mathbf{S}^{-1}. \tag{11}$$

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 β 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 $[\mathrm{H_S} \otimes \mathbb{I}_{\mathrm{B}}, \mathbf{H}_{\mathrm{SB}}] = 0$. 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 α. 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 α and β 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 ($\beta = 0$)

$$\mathbf{H}_{\mathrm{SB}} = \begin{bmatrix} \mathrm{H}_- & \alpha \\ \alpha & \mathrm{H}_+ \end{bmatrix} \quad \text{with} \quad \mathrm{H}_\pm = \omega a^\dagger a \pm (g^* a + g a^\dagger). \tag{12}$$

The operators $\mathrm{H}_\pm$ can be expressed in a more compact form, that is

$$\mathrm{H}_- = \omega \mathrm{D}_f a^\dagger a \mathrm{D}_{-f} - E \quad \text{and} \quad \mathrm{H}_+ = \omega \mathrm{D}_{-f} a^\dagger a \mathrm{D}_f - E, \tag{13}$$

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

$$\text{(i)} \quad \mathrm{D}_{-f} = \mathrm{D}_f^\dagger, \quad \text{(ii)} \quad \mathrm{D}_f \mathrm{D}_{-f} = \mathbb{I}_{\mathrm{B}} \quad \text{and} \quad \text{(iii)} \quad \mathrm{D}_f \mathrm{D}_g = \mathrm{e}^{\mathrm{i}\Im(fg^*)} \mathrm{D}_{f+g}. \tag{14}$$

$\Im$ stands for the imaginary part of the complex number fg^*. Relations (13) can be proven by using equality $\mathrm{D}_f a \mathrm{D}_{-f} = a - f$, 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 $\mathbf{H}_{\mathrm{SB}} \to \mathbf{H}_{\mathrm{SB}} + E$. This is nothing but a rescaling of the reference point of the total.

After this procedure the Hamiltonian (12) takes the form

$$\mathbf{H}_{\mathrm{SB}} = \begin{bmatrix} \omega \mathrm{D}_f a^\dagger a \mathrm{D}_{-f} & \alpha \\ \alpha & \omega \mathrm{D}_{-f} a^\dagger a \mathrm{D}_f \end{bmatrix}, \tag{15}$$

while the corresponding Riccati equation reads

$$\alpha X^2 + X\left(\omega \mathrm{D}_f a^\dagger a \mathrm{D}_{-f}\right) - \left(\omega \mathrm{D}_{-f} a^\dagger a \mathrm{D}_f\right) X - \alpha = 0. \tag{16}$$

To solve this equation, let us first define an operator P_φ in a way that

$$\mathrm{P}_\varphi := \exp(\mathrm{i}\varphi a^\dagger a), \qquad \varphi \in [0, 2\pi). \tag{17}$$

It is not difficult to see that

$$\text{(i)} \quad \mathrm{P}_{-\varphi} = \mathrm{P}_\varphi^\dagger, \quad \text{(ii)} \quad \mathrm{P}_\varphi \mathrm{P}_{-\varphi} = \mathbb{I}_{\mathrm{B}} \quad \text{and} \quad \text{(iii)} \quad \mathrm{P}_\varphi \mathrm{P}_\psi = \mathrm{P}_{\varphi+\psi}. \tag{18}$$

Moreover, from the Baker–Campbell–Hausdorff formula we also have $\mathrm{P}_\varphi a \mathrm{P}_{-\varphi} = \mathrm{e}^{-\mathrm{i}\varphi} a$, which ultimately leads to

$$\mathrm{P}_\varphi \mathrm{D}_f \mathrm{P}_{-\varphi} = \mathrm{D}_{\mathrm{e}^{\mathrm{i}\varphi} f}. \tag{19}$$

In what follows, we will prove that P_π solves the Riccati equation (16). First, let us note that P_π is a function of the number operator $a^\dagger a$, thus $[\mathrm{P}_\pi, a^\dagger a] = 0$. In view of (19) we obtain $\mathrm{P}_\pi \mathrm{D}_f \mathrm{P}_{-\pi} = \mathrm{D}_{-f}$; hence,

$$\mathrm{P}_\pi (\mathrm{D}_f a^\dagger a \mathrm{D}_{-f}) = (\mathrm{D}_{-f} a^\dagger a \mathrm{D}_f) \mathrm{P}_\pi. \tag{20}$$

By writing P_π in terms of the eigenstates $|n\rangle$ of $a^\dagger a$ we obtain

$$\mathrm{P}_\pi = \sum_{n \in \mathbb{N}} \mathrm{e}^{\mathrm{i}\pi n} |n\rangle\langle n| = \sum_{n \in \mathbb{N}} (-1)^n |n\rangle\langle n|, \tag{21}$$

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_π is an involution, i.e. $\mathrm{P}_\pi^2 = \mathbb{I}_{\mathrm{B}}$, which together with (20) leads to

$$\alpha \mathrm{P}_\pi^2 + \mathrm{P}_\pi (\omega \mathrm{D}_f a^\dagger a \mathrm{D}_{-f}) - (\omega \mathrm{D}_{-f} a^\dagger a \mathrm{D}_f) \mathrm{P}_\pi - \alpha = 0. \tag{22}$$

Note, P_π transforms the creation $a^\dagger$ and annihilation a operators into $-a^\dagger$ and $-a$, respectively. In other words, P_π can be interpreted as the bosonic parity operator [38]. Moreover, P_π does not depend on the parameter α; in particular, P_π 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_π, we can derive an accessible form of the time evolution operator $\mathbf{U}_t$. According to (10) and (11) we have

$$\mathbf{U}_t = \frac{1}{2}\begin{bmatrix} U_+(t) & V_+(t)P_\pi \\ V_-(t)P_\pi & U_-(t) \end{bmatrix}, \tag{23}$$

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

$$U_\pm(t) = e^{-i(H_\pm+\alpha P_\pi)t} + e^{-i(H_\pm-\alpha P_\pi)t}, \qquad V_\pm(t) = e^{-i(H_\pm+\alpha P_\pi)t} - e^{-i(H_\pm-\alpha P_\pi)t}. \tag{24}$$

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_π can also be used to construct the constant of motion for the SB model. For this purpose let us take $\mathbf{J}_\pi := \sigma_x \otimes P_\pi$; then $[\mathbf{J}_\pi, \mathbf{H}_{SB}] = 0$, thus from the Heisenberg equations of motion follows $\dot{\mathbf{J}}_\pi = 0$, which means that $\mathbf{J}_\pi$ does not vary with time. Since P_π is an involution, i.e., $P_\pi^2 = \mathbb{I}_B$ thus $\mathbf{J}_\pi$ is an involution as well. Therefore, $\mathbf{J}_\pi$ 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 $H_B \pm V \pm \beta$ are no longer related by an 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:

$$D_f \to \exp(A - A^\dagger), \qquad \text{where} \quad A = \sum_k \frac{g_k^*}{\omega_k} a_k. \tag{25}$$

Then, the solution of the Riccati equation reads

$$P = \exp\left(i\pi \sum_k a_k^\dagger a_k\right) = \bigotimes_k P_{\pi,k}, \quad \text{where} \quad P_{\pi,k} = \exp\left(i\pi a_k^\dagger a_k\right). \tag{26}$$

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

$$\mathrm{Tr}(e^{-i[H_\pm \pm \alpha P_\pi]t} \omega_B \, e^{i[H_\pm \pm \alpha P_\pi]t}) \tag{27}$$

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 $(\mathrm{H}_{\pm} \pm \alpha \mathrm{P}_{\pi})|\psi\rangle = \lambda|\psi\rangle$. 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 $|0\rangle$, $|1\rangle$.

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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