The generalized analytical approximation to the solution of the single-mode spin-boson model without rotating-wave approximation

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Abstract – The single-mode spin-boson model (SMSBM) has extensive application in different subfields of physics. In the absence of rotating-wave approximation (RWA), we try to solve the SMSBM analytically. We argue that the analytical expression obtained might be the most exact approximation to the solution of the system in our case under the assumption of the Abel-Ruffini theorem, which works for a wide range of the parameters such as coupling strength and detuning and would be practical for currently available experiments.

The single-mode spin-boson model (SMSBM), describing a two-level system experiencing a single-mode boson field, is an important prototype in diverse phenomena in almost every subfield of physics. From early day’s studies of the Holstein model [1] in condensed matter physics and the Jaynes-Cummings model [2] in quantum optics to recent investigation of quantum information processing [3,4], the SMSBM has been playing crucial roles.

The rotating-wave approximation (RWA) has been usually employed in treating the SMSBM to simplify the solution under the condition of near resonance and weak coupling, and it could sometimes be successfully applied to some special cases within the characteristic time of the system [5]. However, RWA is not working well any more recently due to experimental availability of strong coupling in atomic system [6], semi-conducting system [7] and superconducting system [8], which implies the necessity of solution to the SMSBM in the absence of RWA.

Without RWA, however, it is hard to have an analytical solution to the SMSBM [9] because the counter-rotating terms make the computational subspace unclosed. As a result, no matter what methods were taken [4,10–16], numerically or semi-analytically, the solutions were made based on the truncated subspace under some special conditions. Alternatively, as the coherent state consists of infinite numbers of Fock states, the computational subspace in the absence of RWA, which is unclosed in the basis of Fock states, could be nearly closed in the coherent-state representation for a wide parameter range. Therefore, employment of coherent states would perhaps enable us to have analytical approximations very close to the exact solution of the problem.

There have been some peculiar characters discovered in the SMSBM without RWA, such as the Bloch-Siegert shift [17], i.e., a shift with respect to the true resonance frequency due to counter-rotating terms, and quantum chaos in cavity QED by differently polarized lights [13]. It has also been shown that the discrepancy of the SMSBM in the presence of RWA with respect to the absence of RWA is reflected by some phase-dependent effects [14]. Most of those discrepancies are meaningful only theoretically, whereas the Bloch-Siegert shift is observable experimentally. For example, in ion traps, the strong laser radiation on the trapped ultracold ions could lead to some level deviation regarding the Bloch-Siegert shift [18–20]. As the laser is usually treated as an external classical light, counter-rotating terms could show observable effects in the blue detuning case. Recent study has demonstrated the possibility of fast logic gating with strong coupling

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between laser and trapped-ion qubits, in which the usual RWA treatment could not work well [21], and the strong nonlinearity would yield considerable complexity in the time evolution [22–24]. As a result, it is of importance to have a more strict study of the SMSBM without RWA.

We have noticed a very recent publication for analytically solving the SMSBM by generalizing the RWA [25]. In the present paper, we will try to explore a more efficient approach to a more generalized analytical result, compared to [25]. The key point is that, by employing the coherent-state representation, we try to diagonalize the matrix regarding the computational subspace. Based on the Abel-Ruffini theorem that no general solution in radicals is possible to polynomial equations of degree five or higher [26], we present analytically the expressions of the energy levels of the system under third-order approximation of the exact wave function, which is relevant to a polynomial equation of degree four. We argue that this might be the most generalized approximation to the solution of the SMSBM under our treatment. To further show the validity of our solution, we will give evidences both analytically and numerically in comparison with the results in previous publications. Moreover, we will show potential application of our result.

Consider following Hamiltonian in units of $\hbar = 1$ [25],

$$H = \begin{pmatrix} \omega_0 a' a + \lambda (a' + a) & \Omega/2 \\ \Omega/2 & \omega_0 a' a - \lambda (a' + a) \end{pmatrix},$$

(1)

where $\Omega$ is the energy splitting of the spin and $\omega_0$ is the frequency of the boson field. $\lambda$ denotes the coupling between the spin and the boson field, and $a$ ($a'$) is the annihilation (creation) operator of the boson field. Equation (1) is taken from [25] in order for us to make comparison between our solution and in [25]. In fact, with respect to the standard quantum optical notation, eq. (1) has been taken a unitary rotation on the two-level system. However, as there is no change of physical essence with that unitary transformation, we will work on eq. (1) in most of this paper.

For convenience of treatment, we may set $g = \lambda/\omega_0$ and employ the displacement operator $D(g) = \exp [g (a' - a)]$ acting on $a'$ and $a$, which yields $A = D(g) a' D(g) = a' + g$, $A' = D(g) a' D(g) = a' + g$, $B = D(-g) a' D(-g) = a' - g$, and $B' = D(-g) a' D(-g) = a' - g$. Consequently, eq. (1) could be rewritten as

$$H_1 = \begin{pmatrix} \omega_0 (A' A - g^2) & \Omega/2 \\ \Omega/2 & \omega_0 (B' B - g^2) \end{pmatrix},$$

(2)

which is formally solvable, and we assume the following trial solution to eq. (2):

$$| \rangle = \sum_{n=0}^{N} (c_n |n\rangle_A |e\rangle + d_n |n\rangle_B |g\rangle),$$

(3)

where $|e\rangle = (1/\sqrt{2})$ and $|g\rangle = (1/\sqrt{2})$, $c_n$ and $d_n$ are coefficients determined later, and $N$ is a large integer relevant to the size of the truncated subspaces. $|n\rangle_{A(B)}$ is a coherent state regarding the operator $A(B)$, which defines as $|n\rangle_A = \frac{1}{\sqrt{n!}} (a' + g)^n |0\rangle_A$ and $|n\rangle_B = \frac{1}{\sqrt{n!}} (a' - g)^n |0\rangle_B$ with $|0\rangle_{A(B)}$ the coherent state in the subspace regarding the operator $A(B)$ [19].

Putting eq. (3) into the Schrödinger equation of eq. (2) would yield

$$\omega_0 (m - g^2) c_m + \frac{\Omega}{2} \sum_{n=0}^{N} (-1)^m D_{mn} d_n = E c_m,$$

(4)

$$\omega_0 (m - g^2) d_m + \frac{\Omega}{2} \sum_{n=0}^{N} (-1)^m D_{mn} c_n = E d_m,$$

(5)

where $(-1)^m D_{mn} = A(m |n\rangle_B, ( -1)^m D_{mn} = B(m |n\rangle_A$, and $D_{mn} = e^{-2g^2 \sum_{k=0}^{m-\min[m,n]} (-1)^k \frac{m! m-n-2k}{(m-k)! (n-k)! k!}}$ [19]. Equations (4) and (5) present the possibility to have a closed solution to the problem. To analytically solve eqs. (4) and (5), we set $d_n = \pm (1)^n c_n$, which yields $\omega_0 (m - g^2) c_m = \frac{\Omega}{2} \sum_{n=0}^{N} D_{mn} c_n = E \pm c_m$. The eigensolution of the equation relies on following determinant:

$$\left| \begin{array}{cccc} \varepsilon_0^\pm & \Omega_{0,1}^\pm & \cdots & \Omega_{0,N}^\pm \\ \Omega_{1,0}^\pm & \varepsilon_1^\pm & \cdots & \Omega_{1,N}^\pm \\ \cdots & \cdots & \cdots & \cdots \\ \Omega_{N,0}^\pm & \Omega_{N,1}^\pm & \cdots & \varepsilon_N^\pm \end{array} \right| = 0,$$

(6)

where $\varepsilon_n^\pm = \omega_0 (m - g^2) + \Omega_{m,m}^\pm - E^\pm = e^\pm - E^\pm$, with $\Omega_{m,n}^\pm = \pm (1/2) \Omega D_{mn}$. As the superscripts $\pm$ are consistent for the relevant variables, the cases regarding superscripts $+$ and $-$ will be treated independently.

In principle, if we consider a large enough value of $N$, eq. (6) would lead us to a nearly exact solution to eqs. (4) and (5). However, in terms of the Abel-Ruffini theorem, to have the analytical results to the best, we have to reduce the determinant to

$$\left| \begin{array}{cccc} \varepsilon_m^\pm & \Omega_{m,m+1}^\pm & \cdots & \Omega_{m,m+3}^\pm \\ \Omega_{m+1,m}^\pm & \varepsilon_{m+1}^\pm & \cdots & \Omega_{m+1,m+3}^\pm \\ \cdots & \cdots & \cdots & \cdots \\ \Omega_{m+3,m}^\pm & \Omega_{m+3,m+1}^\pm & \cdots & \varepsilon_{m+3}^\pm \end{array} \right| = 0,$$

(7)

which leads to a polynomial equation with degree four and should be the most generalized analytical approximation of the solution to the SMSBM under our consideration. Straightforward deduction to eq. (7) yields

see eq. (8) on the next page

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\[
E_m = -\frac{1}{4}(\delta_m + \sqrt{8\chi_m + \delta_m^2 - 4\alpha_m}) - \frac{1}{4}\left(\delta_m + \sqrt{8\chi_m + \delta_m^2 - 4\alpha_m}\right)^2 - 16 \left(\chi_m + \frac{\delta_m\chi_m - \beta_m}{\sqrt{8\chi_m + \delta_m^2 - 4\alpha_m}}\right),
\]

with \( m = 0, 1 \) corresponding to the ground and the first excited states, respectively. Other excited states are

\[
\text{see eq. (9) above}
\]

with \( m = 0, 1, 2, \cdots \), \( \delta_m^\pm = -\sum_{j=0}^3 \epsilon_{m+j} \),

\[
\chi_m^\pm = \left(-q_m^\pm/2 + \sqrt{q_m^\pm^2/4 + \alpha_m^\pm} / 27 \right)^{1/3}
+ \left(-q_m^\pm/2 - \sqrt{q_m^\pm^2/4 + \alpha_m^\pm} / 27 \right)^{1/3} + \alpha_m^\pm / 6,
\]

\[
p_m^\pm = -\alpha_m^\pm \beta_m / 12 + \delta_m^\pm / 4 - \gamma_m^\pm,
\]

\[
q_m^\pm = -\alpha_m^\pm / 108 + \delta_m^\pm \beta_m / 24 + \alpha_m^\pm \gamma_m ^\pm / 3
+ \delta_m^\pm \gamma_m^\pm / 108 + \beta_m^2 / 8,
\]

\[
\alpha_m^\pm = \sum_{j=1}^3 \left(\epsilon_{m+j}^\pm + \epsilon_{m+j+1}^\pm + \Omega_{m+j}^\pm + 3 \Omega_{m+j+1}^\pm - \Omega_{m+j}^\pm - \Omega_{m+j+1}^\pm\right),
\]

\[
\beta_m^\pm = -\sum_{j=0}^3 \left[2 \sum_{k=1}^3 \Omega_{m+j+k}^\pm + 2 \sum_{k=1}^3 \Omega_{m+j+k+1}^\pm + \Omega_{m+j}^\pm + \Omega_{m+j+1}^\pm - \Omega_{m+j+k}^\pm - \Omega_{m+j+k+1}^\pm\right],
\]

and

\[
\gamma_m^\pm = \begin{bmatrix}
\epsilon_m^\pm & \Omega_{m,m+1}^\pm & \Omega_{m,m+2}^\pm & \Omega_{m,m+3}^\pm \\
\Omega_{m+1,m}^\pm & \epsilon_{m+1}^\pm & \Omega_{m+1,m+2}^\pm & \Omega_{m+1,m+3}^\pm \\
\Omega_{m+2,m}^\pm & \Omega_{m+2,m+1}^\pm & \epsilon_{m+2}^\pm & \Omega_{m+2,m+3}^\pm \\
\Omega_{m+3,m}^\pm & \Omega_{m+3,m+1}^\pm & \Omega_{m+3,m+2}^\pm & \epsilon_{m+3}^\pm
\end{bmatrix}.
\]

1We have re-ordered the solutions from the lowest energy to the highest one and also omitted the degenerated levels in order to make a compact and elegant presentation of the result in eqs. (8) and (9). This also holds for the later results for eq. (10).

To prove the validity of eqs. (8) and (9) explicitly, we may work along following two aspects: Comparison with numerical treatment of eq. (6) in the case of a big enough value of \( N \), and comparison with other analytical solutions by the determinants with smaller subspaces. For the former, we have made numerics on eq. (6), as shown in fig. 1, by setting \( N = 42 \) with off-diagonal elements \( \Omega_{ij} \) \((i \text{ or } j \geq N) \) smaller than \( 10^{-6} \). We may assume that numerical result is the exact solution to the problem. Figure 1 shows that our results in eqs. (8) and (9) under the third-order approximation agree with the exact solution very well even in the case that \( \lambda \), \( \Omega \) and \( \omega_0 \) are comparable.

For the latter, we first consider the zeroth-order approximation of eq. (6), i.e., \( \epsilon_m = 0 \), which yields \( E_{m}^\pm = m\omega_0 - (\lambda^2/\omega_0) \pm \Omega D_{mm}/2 \). The first-order approximation
corresponds to
\[
\begin{pmatrix}
  e_m^\pm & \Omega_{m,m+1}^\pm \\
  \Omega_{m+1,m}^\pm & e_{m+1}^\pm
\end{pmatrix} = 0,
\]
which leads to the ground-state energy, \( E_0 = \omega_0(\frac{1}{2} - g^2) - \frac{\Omega^2}{4}(D_{0,0} + D_{1,1}) - \frac{1}{2}\sqrt{[\omega_0 + \Omega^2/2(D_{0,0} - D_{1,1})]^2 + \Omega^2 D_{0,1}^2} \) and the energies for the excited states
\[
E_{k+1}^\pm = \omega_0\left(\frac{1}{2} + k - g^2\right) + (-1)^k \frac{\Omega^2}{4}(D_{k,k} + D_{k+1,k+1}) + \Omega^2 D_{k,k+1}^2,
\]
where \( k = 0, 1, \cdots, N \) and \( D_{k,k+1} = D_{k+1,k} \) is used. It could be found in fig. 2 by comparison with the results in [25] that the excited-state energies we obtain are in good agreement with those in [25], but the ground-state ones are not. In this context, we consider that the results obtained in [25] is basically the one under the first-order approximation in our treatment. But the ground state plotted in [25] seems to be \( E_0 = -\Omega D_{0,0}/2 - \lambda^2/\omega_0 \), i.e., the zeroth-order approximation shown above.

Analogously, we may also obtain the second-order approximation using
\[
\begin{pmatrix}
  e_m^\pm & \Omega_{m,m+1}^\pm & \Omega_{m,m+2}^\pm \\
  \Omega_{m+1,m}^\pm & e_{m+1}^\pm & \Omega_{m+1,m+2}^\pm \\
  \Omega_{m+2,m}^\pm & \Omega_{m+2,m+1}^\pm & e_{m+2}^\pm
\end{pmatrix} = 0,
\]
for which we omit the lengthy expression of the analytical result, but emphasize that the accuracy of the solution depends on how many off-diagonal terms in the determinant of eq. (6) are involved. In general, the farther the off-diagonal elements away from the diagonal line of the matrix in eq. (6), the less important the elements play their roles in the solution. But in the case that \( \Omega, \omega_0 \) and \( \lambda \) are comparable, our numerics shows that the situation is very complicated, for example, \( \Omega_{3,0}, \Omega_{2,0}, \Omega_{0,3}, \Omega_{0,2} \) becoming comparable to \( \Omega_{1,0} \) and \( \Omega_{0,1} \). This is the reason why the omission of elements other than the nearest neighbor to the diagonal terms of the matrix yields the deviation in the mediate coupling case in [25] with respect to the exact solution. In contrast, our treatment could present results more accurate than under the standard RWA and than in [25]. As demonstrated in fig. 1, our analytical expression fits the numerical results very well in a wide range of parameters. Under the assumption of the Abel-Ruffini theorem, we argue that the results we present in eqs. (8) and (9) under the third-order approximation might be the most accurate analytical expression for the energy levels of the SMSBM under our consideration.

Why could we make this? The key reason is the correlation between \( c_n \) and \( d_n \) we found, i.e., \( d_n = (-1)^n c_n \), in the coherent-state representation. What we have done is to try to truncate the Hilbert space appropriately, like in most previous treatments [4,10–16]. But the coherent-state representation helps us to have a nearly close subspace for the solution in the absence of RWA, and the coefficient correlation significantly simplifies our analytical deduction, which makes it available to reach the expression under the third-order approximation.

Compared with purely numerical treatments, our analytical expression, although looks complicated, is actually more easily treated in calculation. Particularly for the large-coupling case, e.g., large values of \( \lambda \) in our case, a numerical solution would have to work in a very large computational subspace, in which most efforts would be paid on keeping convergent in diagonalizing the Hamiltonian of interest. In contrast, our analytical expressions in eqs. (8) and (9) present an effective and efficient treatment to solve the problem under a very good approximation, which avoids the time-consuming diagonalization in any numerics.

On the other hand, our analytical result could present some physics more clearly. For example, for \( n = 0 \) in eq. (3), we have the ground state \( |\rangle = (1/\sqrt{2})(|0\rangle_A|e\rangle - |0\rangle_B|g\rangle) \), which implies that the ground state of the system always overlaps with the upper level of the spin and would always keep evolving if we involve the counterrotating terms in our treatment. In contrast, under the framework of the RWA and even in the generalized RWA treatment [25], the ground state of the system is always uncoupled from other states and thereby remains unchanged no matter how strong the interaction is. Other potential application could also be found in [19].

Furthermore, as our analytical result is very close to the exact solution, we may employ it to study the quantum behavior of the SMSBM under arbitrary conditions.
It seems also possible to apply our method to more complicated situation regarding strong spin-boson coupling. For example, extending the SMSBM to a multi-spin single-mode boson interaction reaches Dicke model [28]. It has been found that the Dicke model in the absence of RWA owes some unique characters [29] with respect to the case in the presence of RWA [30] such as in quantum phase transition, in Berry phase and in entanglement. Moreover, considering the multi-mode boson field, we could relate our solution to another fundamental problem with the environment interrupting a spin-qubit, as shown in a recent work [31], that the Zeno effect is stronger in the absence of RWA than in the presence of RWA, and the anti-Zeno effect disappears if the RWA is removed. With our method by minor modification, we may enable some analytical discussion for the above relevant problems.

In conclusion, we have presented some analytical expressions for solving the SMSBM in the absence of RWA. Although we could not rule out the possibility of another treatment with more accurate approximation by some smart ways, we argue that our third-order approximation might be the most accurate analytical result under our consideration, which could effectively replace the exact numerical solution for studying the SMSBM under arbitrary condition. As the SMSBM has been widely applied to different physical problems [9,32], the coherent-state forms of the eigenfunctions and the analytical expressions of the energy levels of the system would be helpful for understanding the interaction and the dynamics in the spin-boson model under strong coupling or other extreme conditions.

We also conjecture that our technique could be extended to the multi-spin or multi-mode cases. Compared to numerical solutions to these cases, our analytical results would help us to get more physical insight from the complexity.

\[ H' = -\frac{\Omega_0}{2} \sigma_x + \nu a^\dagger a + g(a^\dagger + a)\sigma_z + \epsilon \sigma_x + g^2, \]

where $\Omega_0$ is the Rabi frequency regarding laser-ion coupling, $\nu$ is the trap frequency, $g$ is related to Lamb-Dicke parameter, and $\epsilon$ is the detuning of the laser with respect to the trapped ion. $\sigma_{x,z}$ are usual Pauli operators based on the two levels of the ion [19]. As an example, we demonstrate in Fig. 3 the time evolution of the population in the lower level under the initial condition $\Omega_0/\nu = 1$ or 3/4, $\epsilon = 0$ and $g = 0.8$ with coherent state $\alpha = 1.0$ in vibration. As the results based on eqs. (8) and (9) are nearly the exact solution, we could study the dynamics efficiently from the complicated evolution of the system. The figure also shows the deviation of the results by [25] from the exact dynamics. What is more, as $g = 0.8$ implies the case beyond the Lamb-Dicke limit [19], our analytical results are also useful for understanding the behavior of the ions outside the Lamb-Dicke regime [27] from a purely quantum mechanical viewpoint.

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