Dynamics of Rabi model under second-order Born–Oppenheimer approximation*

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We apply the second-order Born–Oppenheimer (BO) approximation to investigate the dynamics of the Rabi model, which describes the interaction between a two-level system and a single bosonic mode beyond the rotating wave approximation. By comparing with the numerical results, we find that our approach works well when the frequency of the two-level system is much smaller than that of the bosonic mode.

Keywords: Rabi model, second-order Born–Oppenheimer approximation

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1. Introduction

The Jaynes–Cumming model (JCM)[1] which describes the interaction between a two-level system and a single bosonic mode has been studied for decades. With the dipole approximation and rotating wave approximation, this model predicts a wealth of physical phenomenona such as quantum entanglement and coherence.[2–4]

However, the rotating wave approximation is only valid in the case of near-resonant and weak coupling. Nowadays, strong and ultra-strong couplings are realized in polaron-cavity and quantum dot-cavity system.[5,6] Moreover, recent experiments offer an alternative implementation in superconductive quantum circuits instead of the traditional atom–cavity system. For instance, the Cooper-pair box (CPB) interacting with micro-mechanical resonator,[7–9] the flux qubit coupling to the harmonic oscillation[10] or the phase qubit coupling to a nano-mechanical resonator.[11] In these systems, the coupling strength and the detuning are outside the regime of the rotating wave approximation; therefore, the effect arising from the anti-rotating term must be taken into account. In this case, the JCM will be replaced by the Rabi model (which is also called spin-boson model).[12] Up to now, various approximate analytical and numerical approaches have been used to investigate the dynamics of the Rabi system, especially the effect of the anti-rotating wave terms.[13] For example, by the non-blip interacting approximation based on double path integral, the spontaneous emission of the two-level system has been investigated.[12,14] On the other hand, the canonical transformation,[15–19] and the generalized rotating wave approximation (GRWA),[20–22] are applied to derive the effective Hamiltonian in some special conditions. Very recently, an exact approach based on the Bargmann algebra has also been developed, where the eigen energies of the system are obtained by finding the zero points of an analytical function.[23–25]

In this paper, we apply the second-order BO approximation to treat the eigen-problem and the dynamics of the Rabi model. The second-order BO approximation is based on the adiabatic approximation and the detailed derivation is given in Refs. [26] and [27]. The authors have successfully applied the BO approximation to discuss the quantum measurement.[28] We assume that the qubit is prepared in its excited state and the bosonic mode in its vacuum state initially, and focus on the probability of the qubit still in its excited state. Our results agree well with the numerical results when the frequency of the qubit is much smaller than the bosonic mode in both weak and strong couplings.

The paper is organized as follows: In Section 2, we introduce the model and the adiabatic approximation, which is indeed the zeroth-order BO approximation. The second-order approximation is discussed in Section 3. In Section 4, we investigate the dynamical evolution of the system. Some conclusions are drawn in Section 5.

2. Model and zeroth-order Born–Oppenheimer approximation

We generally consider a system consisting of a qubit with the frequency ω_0 and a single bosonic mode with frequency ω. The Hamiltonian of the composite system reads

$$H = \omega a^{\dagger} a + \frac{\omega_0}{2}\sigma_z + g\sigma_x\left(a^{\dagger} + a\right), \tag{1}$$

where $\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|$, $\sigma_x = |0\rangle\langle 1| + |1\rangle\langle 0|$, with $|0\rangle$ and $|1\rangle$ being the excited and ground states of the qubit respectively, $a^{\dagger}$ and a are creation and annihilation operators of the bosonic mode, g is the coupling strength between the qubit and

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the bosonic mode. Many practical physical situations can realize the above system, such as a two-level atom interacting with a single mode optical cavity field, where the coupling strength is weak enough to apply the rotating wave approximation.[3] However, in the circuit QED systems, the coupling strength between the superconductive qubit and the transmission line is much larger[14] and the parameters may achieve far off resonance regime where the frequency of the qubit is much smaller than that of the bosonic mode. In such systems, the traditional rotating wave approximation does not work very well. In the following, we will apply the adiabatic approximation and stationary state perturbation theory to analyze the dynamics of the model.

To solve the dynamics of the Rabi model, we first apply the adiabatic approximation. The main idea of the adiabatic approximation is as follows: if the Hamiltonian of the whole system can be divided into fast variables and slow variables, the fast variables can always modify themselves to acclimatize to the change of the slow variables adiabatically. In other words, for fixed slow variables, the fast variables can induce an effective Hamiltonian. Governed by the effective Hamiltonian, the dynamics of the slow variables can be determined.

In this sense, we assume the frequency of the qubit is much smaller than that of the bosonic mode (i.e., $\omega \gg \omega_0$) and divide the whole Hamiltonian into the slow variables part

$$H_1 = \frac{\omega_0}{2}\sigma_z, \tag{2}$$

and the fast variables part

$$H_2 = \omega a^\dagger a + g\sigma_x\left(a^\dagger + a\right). \tag{3}$$

We now solve the fast variables part. It can be solved through the canonical transformation defined by $\exp(S) = \exp\left[g\sigma_x/\omega\left(a^\dagger - a\right)\right]$, we can obtain the eigenstates as

$$|\psi_n(\pm)\rangle = D\left(\mp\frac{g}{\omega}\right)|n\rangle \otimes |\pm\rangle, \tag{4}$$

and the corresponding eigenenergies are $E_n(\pm) = n\omega - g^2/\omega$, which are two-fold degenerate. In the above equation, $|n\rangle$ is the Fock state of the bosonic mode and $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$ are the eigenstates of σ_x. The displace operators $D[\mp(g/\omega)]$ are defined as

$$D\left(\mp\frac{g}{\omega}\right) = \exp\left[\mp\frac{g}{\omega}(a^\dagger - a)\right]. \tag{5}$$

Within the adiabatic approximation, which is actually the zeroth-order BO approximation, the Hamiltonian in the subspace expanded by the states $\{|\psi_n(+)\rangle, |\psi_n(-)\rangle\}$, can be written as

$$\mathscr{H}_n = \begin{pmatrix} n\omega & \frac{\omega_0}{2}D^+_{nn} \\ \frac{\omega_0}{2}D^-_{nn} & n\omega \end{pmatrix}, \tag{6}$$

the notations $D^\pm_{kn}$ in the above equation are defined as

$$\begin{aligned} D^\pm_{kn} &= \langle k|D^\dagger\left(\pm\frac{g}{\omega}\right)D\left(\mp\frac{g}{\omega}\right)|n\rangle \\ &= \langle k|D\left(\mp\frac{2g}{\omega}\right)|n\rangle. \end{aligned} \tag{7}$$

It is obvious that $D^+_{kn} = (-1)^{k-n}D^-_{kn}$ and we define $D_n \equiv D^+_{nn} = D^-_{nn}$ for simplicity in the following discussion.

The eigen energies of the Hamiltonian $\mathscr{H}_n$ are

$$E_n^{\pm(0)} = n\omega \pm \frac{\omega_0}{2}D_n - \frac{g^2}{\omega}, \tag{8}$$

and the corresponding eigenvectors are

$$\left|\phi_n^{\pm(0)}\right\rangle = \frac{1}{\sqrt{2}}\left(|\psi_n(+)\rangle \pm |\psi_n(-)\rangle\right). \tag{9}$$

3. Second-order Born–Oppenheimer approximation

We have shown that the degeneration is eliminated due to the transition of the qubit between the two eigenstates of σ_x. In the following, we will apply the non-degenerate stationary perturbation theory to obtain the second-order modification for the energy and the first-order modification for the wave function. Before the detailed calculation, we note that the Hamiltonian for the slow variables Eq. (2) not only induce the transition between the states $|\psi_n(+)\rangle$ and $|\psi_n(-)\rangle$, but also between the states $|\psi_n(+)\rangle$ and $|\psi_m(-)\rangle$ for $m \neq n$. However, the amplitude of the latter transition is much smaller than the former one, and is reasonable to treat it as the perturbation part. In this sense, it is reasonable to rewrite the Hamiltonian Eq. (1) as $H = H_0 + H_I$, where

$$\begin{aligned} H_0 &= \sum_n\left(n\omega + \frac{\omega_0}{2}D_n - \frac{g^2}{\omega}\right)\left|\varphi_n^{+(0)}\right\rangle\left\langle\varphi_n^{+(0)}\right| \\ &\quad + \sum_m\left(m\omega - \frac{\omega_0}{2}D_m - \frac{g^2}{\omega}\right)\left|\varphi_m^{-(0)}\right\rangle\left\langle\varphi_m^{-(0)}\right| \end{aligned} \tag{10}$$

is the non-perturbation part H_0 and $H_I = H - H_0$ is the perturbation part.

According to the standard stationary state perturbation theory, we can get the energy up to the second-order and the wave function to the first order. The results can be obtained by straight but complex calculation

$$E_n^\pm = E_n^{\pm(0)} + E_n^{\pm(1)} + E_n^{\pm(2)} \tag{11}$$

and

$$\left|\phi_n^\pm\right\rangle = \left|\phi_n^{\pm(0)}\right\rangle + \left|\phi_n^{\pm(1)}\right\rangle, \tag{12}$$

with $E_n^{\pm(1)} = 0$ and

$$E_n^{\pm(2)} = \frac{\omega_0^2}{16}\sum_{k\neq n}\frac{\left(D^-_{kn} + D^+_{kn}\right)^2}{(n-k)\,\omega \pm (\omega_0/2)\,(D_n - D_k)}$$

$$+\frac{\omega_0^2}{16}\sum_{k\neq n}\frac{\left(D_{kn}^- - D_{kn}^+\right)^2}{(n-k)\,\omega \pm (\omega_0/2)\,(D_n+D_k)}, \tag{13}$$

$$\left|\phi_n^{\pm(1)}\right\rangle = \pm\frac{\omega_0}{4}\sum_{k\neq n}\frac{\left(D_{kn}^- + D_{kn}^+\right)}{(n-k)\,\omega \pm (\omega_0/2)\,(D_n - D_k)}\left|\phi_k^{\pm(0)}\right\rangle \pm\frac{\omega_0}{4}\sum_{k\neq n}\frac{\left(D_{kn}^- - D_{kn}^+\right)}{(n-k)\,\omega \pm (\omega_0/2)\,(D_n+D_k)}\left|\phi_k^{\mp(0)}\right\rangle. \tag{14}$$

The energy levels obtained by our approach (Eq. (11)) and those from the numerical calculations are plotted in Fig. 1. As shown in the figure, when the frequency of the qubit is much smaller than that of the bosonic mode, the second-order BO approximation gives an excellent result. However, when the frequency of the qubit is larger than that of the bosonic mode, our approach loses its effectiveness(not shown in the figure). The same conclusion is also shown in Fig. 2, where we plot the curve of overlap between the wave functions obtained from the numerical result and our approach as a function of the coupling strength g. It is shown that the results from our approach do not coincide with the numerical results even in the resonant case.

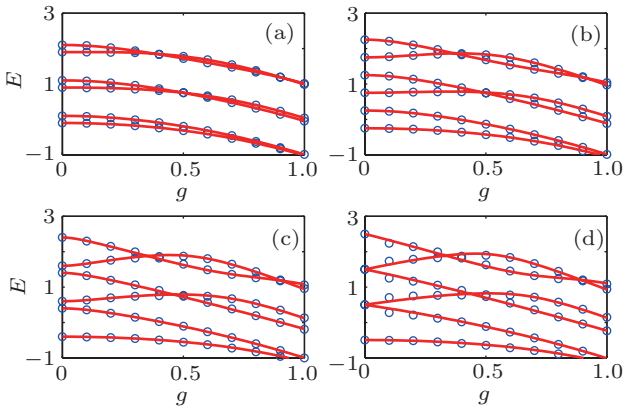


Fig. 1. (color online) The energy spectrum of the system. Red line: the numerical result; Blue circle: the result of second-order BO approximation (Eq. (11)); The parameters are set as $\omega = 1$ and (a) $\omega_0 = 0.2$, (b) $\omega_0 = 0.5$, (c) $\omega_0 = 0.8$, and (d) $\omega_0 = 1$.

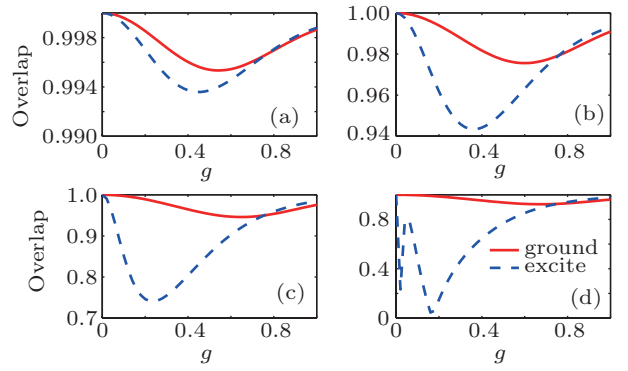


Fig. 2. (color online) The overlap between the wave function obtained in numerical result and second-order BO approximation. The red solid line: the ground state. The blue dashed line: the first excited states. The parameters are set as $\omega = 1$ and (a) $\omega_0 = 0.2$, (b) $\omega_0 = 0.5$, (c) $\omega_0 = 0.8$, and (d) $\omega_0 = 1$.

It shows that, when the frequency of the two-level system is nearly resonant with or larger than that of the bosonic mode, our approach is not valid. The reason can be explained as follows: in the zeroth-order approximation, we regard the free term of the two-level system as a perturbation, which implies that its frequency cannot be too large. In this sense, it is a natural result that our approach is not valid in these situations.

4. Dynamics of system

In the above section, we have obtained the eigen-energy of the system up to the second order and the wave function up to the first order. Based on these results, we will discuss the dynamical evolution of the system.

We assume that the qubit is prepared in its excited state and the bosonic mode is in the vacuum state initially, that is $|\Psi(0)\rangle = |0\rangle_q \otimes |0\rangle_b$. What we are focusing on is the probability $P(t)$ for the qubit still in its excited state after a period of time t.

To this end, we expand the initial state in the basis of the eigenstates as: $|\Psi(0)\rangle = \sum_n a_n |\phi_n^+\rangle + b_n |\phi_n^-\rangle$, where the coefficients a_n and b_n are determined by

$$a_n = \langle\phi_n^+|\Psi(0)\rangle, \tag{15a}$$

$$b_n = \langle\phi_n^-|\Psi(0)\rangle. \tag{15b}$$

Then, at time t, the state of the system becomes

$$|\Psi(t)\rangle = \sum_n a_n \mathrm{e}^{-\mathrm{i}E_n^+ t}\left|\phi_n^+\right\rangle + b_n \mathrm{e}^{-\mathrm{i}E_n^- t}\left|\phi_n^-\right\rangle. \tag{16}$$

In the above equations, $E_n^\pm$ and $\phi_n^\pm$ are defined in Eqs. (11) and (12).

The probability $P(t)$ can then be obtained through the reduced density matrix for the qubit as

$$P(t) = \sum_n \langle 0_q; n\,|\Psi(t)\rangle\langle\Psi(t)\,|0_q; n\rangle. \tag{17}$$

In Fig. 3, we plot the probability $P(t)$ as a function of the evolution time t for different parameters. For comparison, we also plot the results of the zeroth-order BO approximation and those from the numerical calculations. As shown in the figure, when the frequency of the qubit is far off detuning from the bosonic mode, the results of the second-order BO approximation are much more accurate than that of the zeroth order and agree with the numerical results very well for both weak and strong couplings. On the contrary, when the frequency of the qubit is close to that of the bosonic mode, both the zeroth-order and the second-order BO approximation break down.

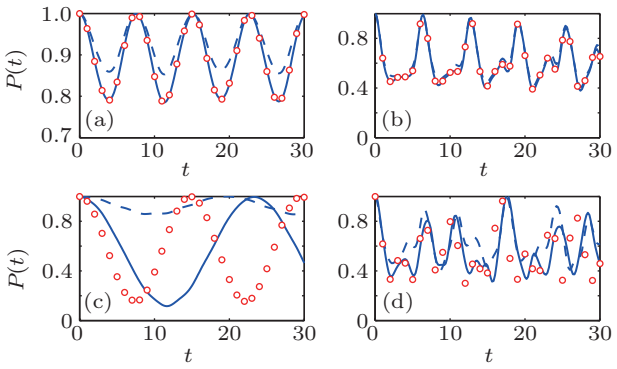


Fig. 3. (color online) The probability of the qubit in its excited state as a function of the evolution time t. The dashed line: the results of the zeroth-order BO approximation. The solid line: the results of the second-order BO approximation. The empty circle: the numerical results. The parameters are set as $\omega = 1$, and (a) $\omega_0 = 0.2$, $g = 0.2$, (b) $\omega_0 = 0.2$, $g = 0.8$, (c) $\omega_0 = 0.8$, $g = 0.2$, and (d) $\omega_0 = 0.8$, $g = 0.8$.

5. Conclusion

In this paper, we study the dynamics of the Rabi model under the second-order BO approximation. To confirm the effectiveness of our approach, we compare our results with the numerical results. We find that the second-order approximation is excellent even for the case of strong couplings when the frequency of the two-level system is much smaller than that of the bosonic mode, where the traditional rotating wave approximation loses its effectiveness. In this regime, the free terms of the two-level system can be safely regarded as a perturbation, and it is natural to obtain a reasonable result.

References

[1] Jaynes E T and Cummings F W 1963 *Proc. IEEE* **51** 89
[2] Raimond J M, Brune M and Haroche S 2001 *Rev. Mod. Phys.* **73** 565
[3] Zheng S B and Guo G C 2000 *Phys. Rev. Lett.* **85** 2392
[4] Walther H, Varcoe B T H, Englert B G and Becker T 2006 *Rep. Prog. Phys.* **69** 1325
[5] Khitrova G, Gibbs H M, Kira M, Koch S W and Scherer A 2006 *Nat. Phys.* **2** 81
[6] Günter G, Anappara A A, Hees J, Sell A, Biasiol G, Sorba L, De Liberato S, Ciuti C, Tredicucci A, Leitenstorfer A and Huber R 2009 *Nat. Lett.* **458** 178
[7] Armour A D, Blencowe M P and Schwab K C 2002 *Physica B* **316** 406
[8] Armour A D, Blencowe M P and Schwab K C 2002 *Phys. Rev. Lett.* **88** 148301
[9] Schoelkopf R J and Girvin S M 2008 *Nat. Lett.* **451** 664
[10] Chiorescu I, Bertet P, Semba K, Nakamura Y, Harmans C J P M and Mooij J E 2004 *Nature* **431** 159
[11] Sornborger A T, Cleland A N and Geller M R 2004 *Phys. Rev. A* **70** 052315
[12] Leggett A J, Chakravarty S, Dorsey A T, Fisher M P A, Garg A and Zwerger W 1987 *Rev. Mod. Phys.* **59** 1
[13] Tang N, Xu T T and Zeng H S 2013 *Chin. Phys. B* **22** 030304
[14] Ishizaki A and Tanimura Y 2008 *Chem. Phys.* **347** 185
[15] Cao X F and Zheng H 2008 *Phys. Rev. A* **77** 022320
[16] Cao X F, You J Q, Zheng H, Kofman A G and Nori F 2010 *Phys. Rev. A* **82** 022119
[17] Gan C J and Zheng H 2010 *Eur. Phys. J. D* **59** 473
[18] Zueco D, Reuther G M, Kohler S and Hänggi P 2009 *Phys. Rev. A* **80** 033846
[19] Yu L X, Zhu S Q, Liang Q F, Chen G and Jia S T 2012 *Phys. Rev. A* **86** 015803
[20] Irish E K, Gea-Banacloche J, Martin I and Schwab K C 2005 *Phys. Rev. B* **72** 195410
[21] Irish E K 2007 *Phys. Rev. Lett.* **99** 173601
[22] Wang Z H, Li Y, Zhou D L, Sun C P and Zhang P 2012 *Phys. Rev. A* **86** 023824
[23] Braak D 2011 *Phys. Rev. Lett.* **107** 100401
[24] He S, Zhang Y Y, Chen Q H, Ren X Z, Liu T and Wang K L 2013 *Chin. Phys. B* **22** 064205
[25] Chen Q H, Li L, Liu T and Wang K L 2012 *Chin. Phys. Lett.* **29** 014208
[26] Sun C P and Ge M L 1990 *Phys. Rev. D* **41** 1349
[27] Sun C P 1995 *Sci. China Ser. A* **38** 224
[28] Sun C P, Liu X F, Zhou D L and Yu S X 2000 *Phys. Rev. A* **63** 012111