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Dynamics of a two-level system coupled to a quantum oscillator: transformed rotating-wave approximation

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Abstract. For studying the dynamics of a two-level system coupled to a quantum oscillator we have presented an analytical approach, the transformed rotating-wave approximation, which takes into account the effect of the counter-rotating terms but still keeps the simple mathematical structure of the ordinary rotating-wave approximation. We have calculated the energy levels of ground and lower-lying excited states, as well as the time-dependent quantum dynamics. It is obvious that the approach is quite simple and can be easily extended to more complicated situation. Besides, the results are compared with the numerically exact ones to show that for weak to intermediate coupling and moderate detuning our analytic calculations are quantitatively in good agreement with the exact ones.

1 Introduction

The physics of a two-level system coupled to a quantum oscillator (spin-oscillator model, SOM) is of wide interest because it provides a simple but ubiquitous model for numerous physical processes, such as the superconducting qubit of Josephson junction [1–6], the semiconductor quantum dot [7,8], the coupling between a qubit and a nanomechanical oscillator [9,10], and a toy model for Holstein polaron [11]. The Hamiltonian of SOM reads

$$H = \frac{1}{2}\Omega\sigma_x + \omega b^\dagger b + \frac{g}{2}\left(b^\dagger + b\right)\sigma_z. \tag{1}$$

Ω is the level difference and σ_x and σ_z are Pauli matrices to describe the two-level system. $b^\dagger$ (b) is the creation (annihilation) operator of the quantum oscillator with frequency ω and g the coupling constant between the two-level system and the oscillator. The model seems quite simple. However, an analytical solution has not yet been found and various approximate analytical and numerical methods have been used.

The Hamiltonian (1) is equivalent to the famous Jaynes-Cummings model with inclusion of both the rotating-wave terms and the counter-rotating terms [12,13],

$$H_{JC} = \frac{1}{2}\Omega\sigma_z + \omega b^\dagger b - \frac{g}{2}\sigma_x\left(b^\dagger + b\right); \tag{2}$$

if a rotation around the y axis is taken for the Pauli matrices, $e^{i\pi\sigma_y/4}\sigma_x e^{-i\pi\sigma_y/4} = \sigma_z$ and $e^{i\pi\sigma_y/4}\sigma_z e^{-i\pi\sigma_y/4} = -\sigma_x$. Then, $b^\dagger$ (b) is the creation (annihilation) operator of the cavity mode and Ω is the atomic transition frequency (g is the vacuum Rabi frequency). Besides, the Hamiltonian (1) is also of interest in the research area of matter-field interaction because it is the following atom-field interaction H_{AF} in the rotating frame [8,14],

$$H_{AF} = \frac{1}{2}\omega_0\sigma_z + \frac{1}{2}\Omega\left(\sigma_+ e^{-i\omega_f t} + \sigma_- e^{i\omega_f t}\right) + \omega b^\dagger b + \frac{g}{2}\left(b^\dagger + b\right)\sigma_z, \tag{3}$$

where $\sigma_\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y)$. Here ω_0 is the atom transition frequency (or the exciton energy in quantum dot) and $\omega_f = \omega_0$ is the frequency of laser field (in resonance with ω_0), and Ω the Rabi frequency. The dynamical evolution of the interacting Hamiltonian H_{AF} can be described by

$$P(t) = \langle\psi_{AF}(t)\left|\sigma_z\right|\psi_{AF}(t)\rangle = \langle\psi(t)\left|\sigma_z\right|\psi(t)\rangle, \tag{4}$$

where $|\psi_{AF}(t)\rangle$ is the wave function of H_{AF} and $|\psi(t)\rangle = e^{i\omega_f t\sigma_z/2}|\psi_{AF}(t)\rangle$ is that of H (Eq. (1)). The initial state of the system is assumed to be $|\psi(0)\rangle = |\psi_{AF}(0)\rangle = |\uparrow\rangle|0\rangle$, where $\sigma_z|\uparrow\rangle = |\uparrow\rangle$ is the eigenstate of σ_z and $|0\rangle$ is the vacuum state of the quantum oscillator. When the coupling $g = 0$ it is easy to get the typical Rabi oscillation $P(t) = \cos(\Omega t)$. For $g \neq 0$, the Rabi oscillation may be modulated by the interaction with the quantum oscillator and it is an interesting problem related to the quantum manipulation of the interacting system [6,10].

Although there is still no analytically exact solution for (1) or (2), various approximate analytical solutions for (1) or (2) already exist [9,10,15–18]. The most popular may be the rotating-wave approximation (RWA), which relies on the assumption of near resonance ($|\Omega - \omega| \ll \Omega$ and ω) and weak coupling ($g \ll \Omega$ and ω). However, the condition of near resonance may not be satisfied if we

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start from Hamiltonian (3), because Ω is the Rabi frequency of the pumping field which may be much larger or smaller than the oscillator frequency [8,14]. Besides, quantum-limited solid-state devices are an alternative to the usual atom-cavity implementation of the SOM, and in these solid-state devices the coupling strength g and the detuning $|\Omega - \omega|$ may be outside the regime where the RWA is valid (the coupling between a nanomechanical resonator and a charge qubit may be in the intermediate range $g/\omega \approx 0.1 \sim 1$ [6,10,18]). This is the motivation for approximate analytical solutions beyond the RWA to be presented in last years.

Recently, Irish [10] proposed an analytical approximate solution for SOM, the generalized RWA which is an improvement to the ordinary RWA. Since a displaced oscillator basis is used to express the Hamiltonian matrix, the generalized RWA is a good approximation for the case of lower Ω ($\Omega \ll \omega$) and/or strong coupling $g/\omega > 1$.

As the Hamiltonian (1) or (2) can be numerically solved easily and quickly by ordinary PC, why do we still need an approximate analytical solution? As far as we can see, the purpose may be: 1) to see the physics more clearly; 2) to test the accuracy of the analytical solution for extending it to more complicated models where a numerically exact solution is difficult to obtain. Hence, we have the following criterion for the validity of an approximate analytical solution: first, it should be as simple as possible, so that it can be easily extended to more complicated situations; second, the main physics should be considered, at least for the interesting and concerned range of the parameters, and it should be as accurate as possible compared with the numerically exact result.

Recently, one of us proposed an analytic approach [19] to the spin-boson model, which describes a two-level system coupled to a dissipative environment [20]. Roughly speaking, Hamiltonian (1) is a simplified version of the spin-boson model, that is, the single mode spin-boson model. Our approach, which is a perturbation expansion based on the unitary transformation, has been successfully applied to several problems related to the interaction between the quantum-limited system and its environment [14,21–24]. In this work, we aim to show the validity of our analytic approach by studying the numerically solvable model, which leads to the transformed rotating-wave approximation (transformed RWA) for model (1). We will focus on the dynamical evolution $P(t)$, since the accuracy of its calculation depends not only on the calculation of ground state but also on that of the lower-lying excited states. The dynamical evolution $P(t)$ calculated by our transformed RWA will be compared to the numerically exact one, as well as to the ordinary RWA, to show that for weak to intermediate coupling and moderate detuning our calculations are quantitatively in good agreement with the numerically exact results.

2 Theoretical analysis

The ordinary RWA for the SOM (Eq. (1)) is

$$H_{RWA} = \frac{1}{2}\Omega\sigma_x + \omega b^\dagger b + \frac{g}{2}\left[b^\dagger|s_1\rangle\langle s_2| + b|s_2\rangle\langle s_1|\right], \quad (5)$$

where $\sigma_x|s_1\rangle = -|s_1\rangle$ and $\sigma_x|s_2\rangle = |s_2\rangle$ are the eigenstates of σ_x. It is easy to see that $|s_1\rangle|0\rangle$ ($|0\rangle$: the vacuum state of the oscillator) is the exact ground state of H_{RWA} and the mathematical structure of H_{RWA} is quite simple.

We apply a unitary transformation [19] to H (Eq. (1)), $H' = \exp(S)H\exp(-S)$, and the purpose of the transformation is to take into account the effect of counter-rotating terms, where

$$S = \frac{g}{2\omega}\xi\sigma_z\left(b^\dagger - b\right). \quad (6)$$

A parameter ξ is introduced in S and its form will be determined later. The transformation can be done to the end and the result is

$$H' = H'_0 + H'_1 + H'_2, \quad (7)$$

$$H'_0 = \frac{1}{2}\eta\Omega\sigma_x + \omega b^\dagger b - \frac{g^2}{4\omega}\xi(2-\xi), \quad (8)$$

$$H'_1 = \frac{1}{2}g(1-\xi)\left(b^\dagger + b\right)\sigma_z + \frac{1}{2}\eta\Omega i\sigma_y\frac{g}{\omega}\xi\left(b^\dagger - b\right), \quad (9)$$

$$H'_2 = \frac{1}{2}\Omega\sigma_x\left(\cosh\left\{\frac{g}{\omega}\xi\left(b^\dagger - b\right)\right\} - \eta\right) + \frac{1}{2}\Omega i\sigma_y\left(\sinh\left\{\frac{g}{\omega}\xi\left(b^\dagger - b\right)\right\} - \eta\frac{g}{\omega}\xi\left(b^\dagger - b\right)\right), \quad (10)$$

where η is determined by the following vacuum average,

$$\eta = \langle 0|\cosh\left\{\frac{g}{\omega}\xi\left(b^\dagger - b\right)\right\}|0\rangle = \exp\left[-\frac{g^2}{2\omega^2}\xi^2\right]. \quad (11)$$

Obviously, H'_0 can be solved exactly because for which the spin and the oscillator are decoupled. If the displacement parameter ξ is determined as

$$\xi = \frac{\omega}{\omega + \eta\Omega}, \quad (12)$$

then we have

$$H'_1 = \frac{1}{2}\eta\Omega\frac{g}{\omega}\xi\left[b^\dagger\left(\sigma_z + i\sigma_y\right) + b\left(\sigma_z - i\sigma_y\right)\right] = \eta\Omega\frac{g}{\omega}\xi\left[b^\dagger|s_1\rangle\langle s_2| + b|s_2\rangle\langle s_1|\right]. \quad (13)$$

Note that H'_1 is of the same form as the RWA in equa-

$O(g^4)$. This means that through the unitary transformation we get the transformed RWA Hamiltonian H_{TRWA}, which is of the same mathematical structure as the ordinary RWA H_{RWA} in (5). $|g_0\rangle = |s_1\rangle|0\rangle$ is also the exact ground state of H_{TRWA} (because of $H_1'|g_0\rangle = 0$) with ground state energy

$$E_g = -\frac{1}{2}\eta\Omega - \frac{g^2}{4\omega}\xi(2-\xi). \tag{14}$$

The eigenenergy for excited states can be easily obtained from H_1' (Eq. (13)), since it contains the rotating-wave terms only. For $n = 0, 1, 2, ...$, the eigenenegies for all excited states are

$$E_{2n+1} = \left(n+\frac{1}{2}\right)\omega - \frac{1}{2}\sqrt{(\omega-\eta\Omega)^2 + g'^2(n+1)} - \frac{g^2}{4\omega}\xi(2-\xi), \tag{15}$$

$$E_{2n+2} = \left(n+\frac{1}{2}\right)\omega + \frac{1}{2}\sqrt{(\omega-\eta\Omega)^2 + g'^2(n+1)} - \frac{g^2}{4\omega}\xi(2-\xi), \tag{16}$$

where $g' = 2g\eta\Omega/(\omega+\eta\Omega)$. We note that when we are close to resonance at $\omega \approx \eta\Omega$, $g' \approx g$, and H_{TRWA} is nearly the same as H_{RWA} except an overall energy shift $-g^2\xi(2-\xi)/4\omega$ coming from our unitary transformation. This is to say that close to resonance H_{TRWA} is as good as H_{RWA} (but with better evaluation of ground state energy, see Eq. (14)). Hence, in the following we will mainly consider the off-resonance case.

The calculations of the ground state and lower-lying excited states with moderate detuning are shown in Figures 1 and 2. Figure 1 is for the case of $\Omega = 1$ and $\omega = 0.5$; Figure 2 for $\Omega = 0.5$ and $\omega = 1$. For comparison, the results of exact diagonalization and those of generalized RWA [10] are also shown. For ground state energy our result of transformed RWA is very close to the exact result and is better than that of generalized RWA. For excited states we could not say definitely which one is better, but we can say that for intermediate coupling $g/\omega \approx 0.1 \sim 1$ our results of transformed RWA are quite close to the exact results.

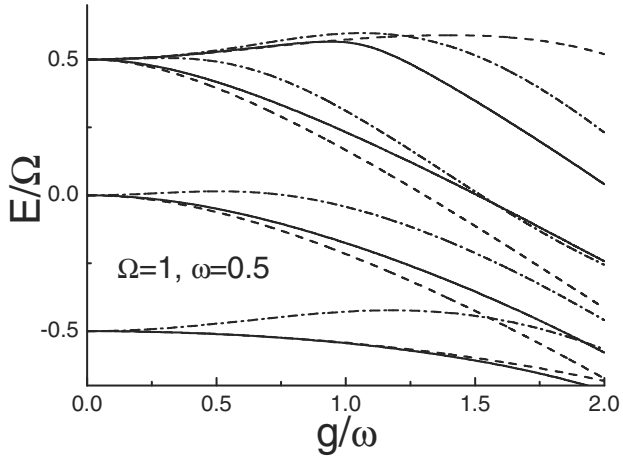

Fig. 1. The energy levels of the ground state (E_g) and the lower-lying excited states (E_1, E_2 and E_3, from bottom to top) as functions of the ratio g/ω. $\Omega = 1$ and $\omega = 0.5$. Our results (dashed lines) are compared with the numerically exact ones (solid lines) and those of the GRWA reference [10] (dashed-dotted lines).

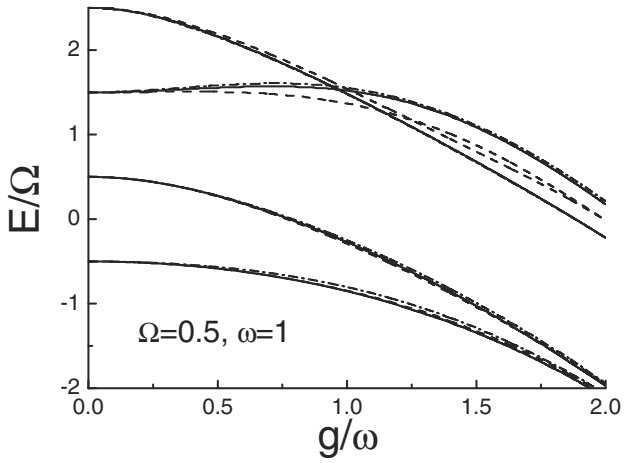

Fig. 2. The energy levels of the ground state (E_g) and the lower-lying excited states (E_1, E_2 and E_3, from bottom to top) as functions of the ratio g/ω. $\Omega = 0.5$ and $\omega = 1$. Our results (dashed lines) are compared with the numerically exact ones (solid lines) and those of the GRWA reference [10] (dashed-dotted lines).

3 Dynamical evolution P(t)

We have shown that for the weak to intermediate coupling our calculation of the ground state and the lower-lying excited state is quantitatively in good agreement with the numerically exact results, which is a check of the validity of our approach. Furthermore, in this section our approach will be checked by calculation of the excited state properties, that is, the dynamical evolution $P(t)$ of equation (4).

The numerical exact calculation for $P(t)$ with Hamiltonian H can be obtained by the numerical diagonalization. The following is the calculation of $P(t)$ in our transformed RWA. From equation (4) we have

$$\begin{aligned} P(t) &= \langle\psi(0)|e^{iHt}\sigma_z e^{-iHt}|\psi(0)\rangle \\ &= \langle\psi(0)|e^{-S}e^{iH't}e^{S}\sigma_z e^{-S}e^{-iH't}e^{S}|\psi(0)\rangle \\ &\approx \langle\psi'(0)|\exp(iH_{TRWA}t)\,\sigma_z\exp(-iH_{TRWA}t)|\psi'(0)\rangle \\ &= \langle\psi_I'(t)|e^{iH_0't}\sigma_z e^{-iH_0't}|\psi_I'(t)\rangle, \end{aligned} \tag{17}$$

where $|\psi'(0)\rangle = e^S|\psi(0)\rangle$. Here the unitary transformations, $e^S H e^{-S} = H'$ and $e^S\sigma_z e^{-S} = \sigma_z$, have been used. $|\psi_I'(t)\rangle = e^{iH_0't}\exp(-iH_{TRWA}t)|\psi'(0)\rangle$ is the wave

function in interaction picture, which is the solution of following Schroedinger equation,

$$i\frac{\partial}{\partial t}|\psi_I'(t)\rangle = H_1'(t)|\psi_I'(t)\rangle, \tag{18}$$

$$H_1'(t) = e^{iH_0't}H_1'e^{-iH_0't} = \frac{g'}{2}\left(b^\dagger|s_1\rangle\langle s_2|e^{i(\omega-\eta\Omega)t}+b|s_2\rangle\langle s_1|e^{-i(\omega-\eta\Omega)t}\right). \tag{19}$$

The initial state is $|\psi'(0)\rangle = e^S|\uparrow\rangle|0\rangle = \frac{1}{\sqrt{2}}(|s_1\rangle + |s_2\rangle)e^{\alpha(b^\dagger-b)}|0\rangle$ with $\alpha = g\xi/2\omega$. Here the exponential operator is expanded to the order α: $e^{\alpha(b^\dagger-b)} \approx 1+\alpha(b^\dagger-b)$ and, hence, the initial condition is

$$C_{10}(0) = C_{20}(0) = \frac{1}{\sqrt{2}},$$
$$C_{11}(0) = C_{21}(0) = \frac{\alpha}{\sqrt{2}}, \quad C_{12}(0) = 0, \tag{20}$$

with the wave function [25]

$$|\psi_I'(t)\rangle = C_{10}(t)|s_1\rangle|0\rangle + C_{20}(t)|s_2\rangle|0\rangle + C_{11}(t)|s_1\rangle|1\rangle + C_{21}(t)|s_2\rangle|1\rangle + C_{12}(t)|s_1\rangle|2\rangle. \tag{21}$$

The Schroedinger equation is [25]

$$i\frac{d}{dt}C_{10}(t) = 0, \tag{22}$$

$$i\frac{d}{dt}C_{20}(t) = \frac{g'}{2}e^{i(\eta\Omega-\omega)t}C_{11}(t),$$
$$i\frac{d}{dt}C_{11}(t) = \frac{g'}{2}e^{-i(\eta\Omega-\omega)t}C_{20}(t), \tag{23}$$
$$i\frac{d}{dt}C_{21}(t) = \frac{g'}{2}e^{i(\eta\Omega-\omega)t}C_{12}(t),$$
$$i\frac{d}{dt}C_{12}(t) = \frac{g'}{2}e^{-i(\eta\Omega-\omega)t}C_{21}(t). \tag{24}$$

Then, the solution for equation (23) is

$$C_{20}(t) = \frac{1}{\sqrt{2}}\left\{\left[\cos\frac{\Phi_0 t}{2} - i\frac{\eta\Omega-\omega}{\Phi_0}\sin\frac{\Phi_0 t}{2}\right] - \alpha\frac{ig'}{\Phi_0}\sin\frac{\Phi_0 t}{2}\right\}e^{i(\eta\Omega-\omega)t/2}, \tag{25}$$

$$C_{11}(t) = \frac{1}{\sqrt{2}}\left\{\alpha\left[\cos\frac{\Phi_0 t}{2} + i\frac{\eta\Omega-\omega}{\Phi_0}\sin\frac{\Phi_0 t}{2}\right] - \frac{ig'}{\Phi_0}\sin\frac{\Phi_0 t}{2}\right\}e^{-i(\eta\Omega-\omega)t/2}, \tag{26}$$

and the solution for equation (24) is

$$C_{21}(t) = \frac{\alpha}{\sqrt{2}}\left[\cos\frac{\Phi_1 t}{2} - i\frac{\eta\Omega-\omega}{\Phi_1}\sin\frac{\Phi_1 t}{2}\right]e^{i(\eta\Omega-\omega)t/2}, \tag{27}$$

$$C_{12}(t) = -\frac{\alpha}{\sqrt{2}}\frac{i\sqrt{2}g'}{\Phi_1}\sin\frac{\Phi_1 t}{2}e^{-i(\eta\Omega-\omega)t/2}, \tag{28}$$

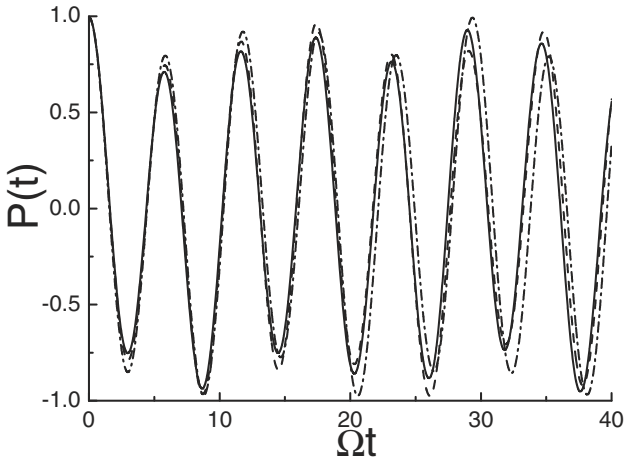

Fig. 3. Time evolution $P(t)$ for $\Omega = 1$, $\omega = 0.5$ and $g = 0.4$. The dashed line is our transformed RWA calculation. The solid line and the dashed-dotted line are the numerically exact result and the ordinary RWA one, respectively.

where $\Phi_0^2 = (\eta\Omega-\omega)^2 + g'^2$ and $\Phi_1^2 = (\eta\Omega-\omega)^2 + 2g'^2$. The dynamical evolution is

$$P(t) = 2\mathrm{Re}\left(C_{20}^*(t)C_{10}(t)e^{i\eta\Omega t} + C_{21}^*(t)C_{11}(t)e^{i\eta\Omega t}\right). \tag{29}$$

For the ordinary RWA (Eq. (5)), the interaction is

$$H_1(t) = \frac{g}{2}\left(b^\dagger|s_1\rangle\langle s_2|e^{i(\omega-\Omega)t} + b|s_2\rangle\langle s_1|e^{-i(\omega-\Omega)t}\right). \tag{30}$$

Then, it is easily to get the dynamical evolution,

$$P_{RWA}(t) = \cos\frac{\Phi_{0,RWA}t}{2}\cos\frac{(\Omega+\omega)t}{2} - \frac{\Omega-\omega}{\Phi_{0,RWA}}\sin\frac{\Phi_{0,RWA}t}{2}\sin\frac{(\Omega+\omega)t}{2}, \tag{31}$$

where $\Phi_{0,RWA}^2 = (\Omega-\omega)^2 + g^2$.

The calculations of $P(t)$ with moderate detuning and intermediate coupling are shown in Figures 3 and 4. Figure 3 is for the larger Ω case ($\Omega = 1$, $\omega = 0.5$ and $g = 0.4$); Figure 4 for larger ω case ($\Omega = 0.5$, $\omega = 1$, and $g = 0.5$). For comparison, the results of exact diagonalization and those of ordinary RWA are also shown. one can see that our results of transformed RWA are quite close to the numerically exact ones, much better than those of ordinary RWA (especially for the case of Fig. 4).

For some special cases the ordinary RWA is absolutely invalid. Figure 5 shows the $P(t)$ dynamics for large detuning $\omega = 1$, $\Omega = 0.25$ and strong coupling $g = 1$. One can see that the result of ordinary RWA is qualitatively incorrect, but that of our transformed RWA is still in qualitative agreement with the numerically exact one.

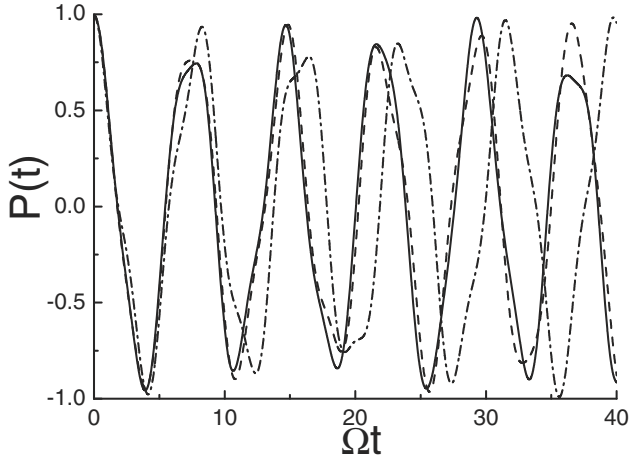

Fig. 4. Time evolution $P(t)$ for $\Omega = 0.5$, $\omega = 1$ and $g = 0.5$. The dashed line is our transformed RWA calculation. The solid line and the dashed-dotted line are the numerically exact result and the ordinary RWA one, respectively.

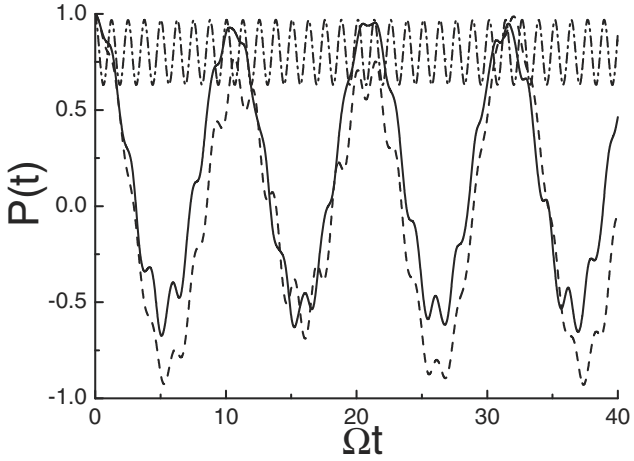

Fig. 5. Time evolution $P(t)$ for $\Omega = 0.25$, $\omega = 1$ and $g = 1$. The dashed line is our transformed RWA calculation. The solid line and the dashed-dotted line are the numerically exact result and the ordinary RWA one, respectively.

4 Concluding remarks

We have presented an analytical approach, the transformed RWA, for the SOM, which takes into account the effect of counter-rotating terms but still keeps the simple mathematical structure of the ordinary RWA. We have investigated the energy levels of ground and lower-lying excited states, as well as the time-dependent quantum dynamics. It is obvious that the approach is quite simple and can be easily extended to more complicated situation. Besides, the results are compared with the numerically exact ones to show that for weak to intermediate coupling and moderate detuning our analytic calculations are quantitatively in good agreement with the exact ones.

The key point of our treatment is the unitary transformation with generator S, where a parameter $\xi = \omega/(\omega + \eta\Omega)$ is introduced. The "speed" of atom is Ω and the "speed" of oscillator is ω. When $\omega \gg \Omega$, the oscillator can follow the atom adiabatically and $\xi \approx 1$. In this region the generalized RWA of reference [10] works well since it is good for higher frequency $\omega \gg \Omega$ and strong coupling $g/\omega \gg 1$. When $\omega \ll \Omega$, the oscillator cannot follow the atom and $\xi \ll 1$, that is, an ordinary perturbation treatment may be good enough if the interaction is not strong. Our choice of $0 < \xi < 1$ is in between to take into account the nonadiabatic effect when the retardation of the interaction between the atom and the quantum oscillator with moderate detuning and intermediate coupling is important. In addition, the bare coupling g in original Hamiltonian H is replaced by the renormalized coupling $g' = 2g\eta\Omega/(\omega + \eta\Omega)$ in H_{TRWA} because the effect of the counter-rotating terms has been included.

Finally, we can check how "large" the dropped H_2' is by calculating its contribution to the ground state energy. First, we already showed that equation (11) leads to $\langle g_0|\tilde{H}_2|g_0\rangle = 0$. Second, because of the chosen form of η we can prove that $\langle g_0|\tilde{H}_2|s_2\rangle|0\rangle = 0$, $\langle g_0|\tilde{H}_2 b^\dagger|g_0\rangle = 0$, and $\langle g_0|\tilde{H}_2 b^\dagger|s_2\rangle|0\rangle = 0$. So, the lowest-order nonzero matrix element is $\langle g_0|\tilde{H}_2 b^\dagger b^\dagger|g_0\rangle = -0.5\eta\Omega g^2/(\omega + \eta\Omega)^2$. Then, the lowest-order correction to the ground state energy is

$$-\frac{\left|\langle g_0|\tilde{H}_2 b^\dagger b^\dagger|g_0\rangle\right|^2}{2\omega} = \frac{\omega}{8}\eta^2\frac{g^4}{(\omega+\eta\Omega)^4},$$

which is of the order of g^4.

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