THE RABI HAMILTONIAN IN THE DISPERSIVE REGIME*

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The Rabi Hamiltonian is studied in the dispersive regime and ultra-strong coupling. We employ a recent unitary transformation to obtain not only the approximate Hamiltonian and its energy levels but also its eigenfunctions. The relationship of the approximation with other regimes and their approximations are also discussed.

Key words: Two-level system, qubit, Rabi model, Jaynes-Cummings model.

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1. INTRODUCTION

The Rabi Hamiltonian was used initially to describe the interaction of nuclear spins with magnetic fields [1], but it is also used to model the ammonia molecule [2] or electrons coupled with a phonon mode in a crystal lattice [3]. More recently, beside the interaction of atoms with an electromagnetic field in a cavity [4] the Rabi Hamiltonian describes the interaction of superconducting qubits with a nanomechanical resonator [5], with a transmission line resonator [6], or an LC resonator [7]. The Rabi Hamiltonian expresses the interaction of a two-level system (TLS) with a single boson mode and has the following form:

$$H = \omega a^{\dagger} a + \Omega \sigma_z + \lambda (a^{\dagger} + a)(\sigma_- + \sigma_+), \tag{1}$$

where $\hbar = 1$, σ_x, σ_y, and σ_z are spin $1/2$ matrices, $\sigma_{\pm} = \sigma_x \pm i\sigma_y$, $a^{\dagger}$ and a are the creation and annihilation operators of the quantum oscillator.

The apparent simplicity of (1) led to the conjecture about its solvability [8] that only recently has been fully proved [9]. Despite the fact that the Rabi Hamiltonian is completely solvable, its general solutions cannot be easily grasped in simple terms. In quantum optics with atoms in a cavity also known as cavity quantum electrodynamics (cavity QED) one encounters a regime of quasi-resonance ($\omega \approx \Omega$) and a coupling strength λ/ω between 10^{-7} and 10^{-5}. This regime is very well described by the Jaynes-Cummings model which is simpler and solvable [10]. The Jaynes-Cummings

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model uses the rotating wave approximation (RWA) in (1), such that the counter-rotating wave term $a^{\dagger}\sigma_{+}+a\sigma_{-}$ is completely ignored [4]. Moreover, in the circuit QED [5–7, 12], where the TLS is associated with a qubit, one encounters a dispersive regime (*i.e.*, large detuning $|\omega-\Omega|\sim\omega+\Omega$) with a ultra-strong coupling $\lambda/\omega\sim 0.1$, where the Jaynes-Cummings model fails [13–15]. A more elaborate approximation based on the polaron transformation [3, 16] is the generalized RWA, which works well in the region of zero and large detuning and ultra-strong coupling [11].

Recently, Zueco *et al.* [17] used the same technique of the unitary transformations to include the counter-rotating wave term with an improved accuracy of energy levels for a wider range of parameters. We build on that work and in Section 2 we provide not only the approximate Hamiltonian and its eigenvalues but also its eigenfunctions to the second order in the coupling constant. In section 3 we discuss comparatively the regimes of slow and fast TLS with respect to the oscillator and in Section 4 we conclude the work.

2. THE APPROXIMATE HAMILTONIAN IN THE DISPERSIVE REGIME

Quite often a general Hamiltonian H can be decomposed as $H=H_0+\lambda W$, where H_0 is diagonalizable and λ is a small real parameter. The ultimate goal of the unitary transformation approach is to find an anti-hermitian operator S such that the unitary transformation $U=e^{\lambda S}$ diagonalizes H. However, the complete diagonalizing is not always possible but it can be done successively beginning with the first order of λ. The requirement to eliminate λW in the first order leads to the form of S that is given by $S=-i\lambda\lim\limits_{\varepsilon\to 0_{+}}\int\limits_{-\infty}^{0}e^{\varepsilon t}W_{I}(t)\,dt$, where $W_{I}(t)=e^{iH_{0}t}We^{-iH_{0}t}$ [18]. If we choose $H_0=\omega a^{\dagger}a+\Delta\sigma_z$ and $\lambda W=\lambda\left(a+a^{\dagger}\right)\left(\sigma_{-}+\sigma_{+}\right)$ we can calculate S as being

$$S=-\frac{2i\omega}{\Delta^{2}-\omega^{2}}\left(\frac{a-a^{\dagger}}{i}\right)\sigma_{x}-\frac{2i\Delta}{\Delta^{2}-\omega^{2}}\left(a+a^{\dagger}\right)\sigma_{y}. \tag{2}$$

The use of (2) in the transformation $U_1=e^{\lambda S}$ changes the Rabi Hamiltonian into

$$\tilde{H}=\omega a^{\dagger}a+\Delta\sigma_{z}+\frac{2\lambda^{2}\Delta}{\Delta^{2}-\omega^{2}}\left(a+a^{\dagger}\right)^{2}\sigma_{z}+\frac{\lambda^{2}\omega}{\Delta^{2}-\omega^{2}}+O\left(\lambda^{3}\right). \tag{3}$$

We notice that the small parameter is $\tilde{\lambda}=\lambda^{2}/(\Delta^{2}-\omega^{2})$ and if $\tilde{\lambda}\ll 1$ we can retain just the first three terms of (3). Then we expand $\left(a+a^{\dagger}\right)^{2}$, make some arrangements and remove completely the part of Hamiltonian proportional with $a^{2}+{a^{\dagger}}^{2}$. This is possible with the unitary transformation $U_2=e^{\hat{\beta}\sigma_{z}(a^{2}-{a^{\dagger}}^{2})}$, where $\hat{\beta}=\begin{pmatrix}\beta_{+} & 0\\ 0 & \beta_{-}\end{pmatrix}$

and $tanh(2\beta_{\pm}) = \frac{\pm 2\tilde{\lambda}\Delta}{\omega \pm 2\tilde{\lambda}\Delta}$. Thus, the approximate form of (3) is

$$H_1 = a^{\dagger}a\sqrt{\omega^2 + 8\tilde{\lambda}\omega\Delta\sigma_z} + \frac{\sqrt{\omega^2 + 8\tilde{\lambda}\omega\Delta\sigma_z} - \omega}{2} + (1+2\tilde{\lambda})\Delta\sigma_z + \tilde{\lambda}\omega. \quad (4)$$

To be fully consistent with the approximations made so far we expand the radical in Eq. (4) and keep just the first two terms in the series. Thus, the oscillator frequencies are $\omega_{\pm} = \omega \pm 2\tilde{\lambda}\Delta$ and the Hamiltonian (4) turns into the Hamiltonian of the dispersive regime and ultra-strong coupling

$$H_{approx} = a^{\dagger}a \begin{pmatrix} \omega_+ & 0 \\ 0 & \omega_- \end{pmatrix} + (1+4\tilde{\lambda})\Delta\sigma_z + \tilde{\lambda}\omega. \quad (5)$$

It is easy to see that the eigenvalues of (5) are

$$E_{\pm n} = n\omega_{\pm} \pm \frac{1+4\tilde{\lambda}}{2}\Delta + \tilde{\lambda}\omega. \quad (6)$$

We also calculate the eigenvectors of (5) in the original Schrödinger picture. In order to do so we need to evaluate the action of $e^{\lambda S}$ on any vector in the Hilbert space of the problem. The action of $e^{\lambda S}$ is rather cumbersome but a meaningful expression can be obtained with the Zassenhaus formula [19], which, for any operator A and B reads $e^{\lambda(A+B)} = e^{\lambda A}e^{\lambda B}e^{-\frac{\lambda^2}{2}[A,B]}\ldots$. Thus, the eigenvectors of (5) are

$$|\Psi_{\pm n}> = e^{-i\frac{2\lambda\omega}{\Delta^2-\omega^2}\frac{a-a^{\dagger}}{i}\sigma_x} e^{-i\frac{2\lambda\Delta}{\Delta^2-\omega^2}(a+a^{\dagger})\sigma_y} e^{(\frac{2\lambda^2\omega\Delta}{(\Delta^2-\omega^2)^2}+\hat{\beta})(a^2-a^{\dagger 2})\sigma_z} |n(\omega_{\pm})> s_{\pm}. \quad (7)$$

In Eqs. (6) and (7) n is a natural number, $|n(\omega_{\pm})>$ are the nth eigenvectors of the quantum oscillator with frequencies $\omega_{\pm}$, and $s_{\pm}$ are the eigenvectors of σ_z, *i.e.*, $\sigma_z s_{\pm} = (\pm 1/2)s_{\pm}$.

3. DISCUSSIONS

The energy levels given by Eq. (6) have been compared with the exact eigenvalues of (1) in the paper of Zueco *et al.* [17], where it has been proved a very good match between (6) and the eigenvalues of (1) for a wide range of parameters in the dispersive regime. On the other hand, the accuracy of eigenfunctions has been checked in Ref. [20] by calculating their fidelity with respect to the exact numerical calculated eigenfunctions. The comparison of the eigenfunctions have been performed in two limiting cases of the dispersive regime: slow TLS and fast oscillator ($\Delta \ll \omega$) and slow oscillator and fast TLS ($\Delta \gg \omega$).

In the slow TLS and fast oscillator regime ($\Delta \ll \omega$) Agarwal *et al.* [20] have found that the eigenvectors of Hamiltonian (5) in Schrödinger picture have a poor

fidelity with respect to the exact eigenvectors. Moreover, their calculations indicated that the fidelity of the eigenvectors provided by the adiabatic approximation [11, 16] is excellent. We compare our results given by (7) with the adiabatic eigenvectors. We recall that the adiabatic approximation is obtained using the polaron transformation $e^{2\frac{\lambda}{\omega}(a-a^\dagger)\sigma_x}$ and neglecting the spin non-diagonal term [16]. Hence, the adiabatic Hamiltonian and its eigenvectors are, respectively,

$$H_{adiab} = \omega a^\dagger a + \Delta\sigma_z cos(\frac{2\lambda}{\omega}\frac{a-a^\dagger}{i}) - \frac{\lambda^2}{\omega}, \tag{8}$$

$$|\Psi_{\pm n\_adiab}>= e^{2\frac{\lambda}{\omega}(a-a^\dagger)\sigma_x}|n(\omega)> s_\pm. \tag{9}$$

When $\Delta \ll \omega$ both λ/ω and Δ/ω are small, therefore (7) becomes

$$|\Psi_{\pm n}>= e^{\frac{2\lambda}{\omega}(a-a^\dagger)\sigma_x} e^{2i\frac{\lambda\Delta}{\omega^2}(a+a^\dagger)\sigma_y} e^{\frac{\lambda^2\Delta}{\omega^3}(a^2-a^{\dagger 2})(2\sigma_z+1)}|n(\omega_\pm)> s_\pm \tag{10}$$

In Eq. (10) the part that contains the squeeze operator deviates from the unit operator by an amount of the same order as the overlap $< n(\omega)|n(\omega_\pm) >$ differs from unity, *i.e.*, $O(\frac{\lambda^2\Delta}{\omega^3})$, thus their deviation from 1 can be safely discarded. It is easy now to evaluate the fidelity between (9) and (10) as $f = | < \Psi_{\pm n\_adiab}|\Psi_{\pm n} > |^2 = 1 - O(\frac{\lambda\Delta}{\omega^2})$, which it is very close to 1. It would imply that the fidelity of (7) is close to one, which is in stark contrast with Ref. [20]. One possible explanation of this discrepancy might be the way $e^{\lambda S}$ is calculated to obtain the eigenfunctions. We adopted an exponential approximation based on the Zassenhaus formula, but if one adopts a series expansion of $e^{\lambda S}$, the fidelity would be $f = 1 - O(\lambda/\omega)$, which is sensibly below unity and consistent with the conclusions of Agarwal *et al.*

In the region $\Delta \gg \omega$ (fast TLS and slow oscillator) one can also invoke an adiabatic approximation as long as the TLS and the oscillator are on two different energy scales. This situation is more often encountered in molecules and crystals [2]. The new adiabatic regime can be obtained by a unitary transformation that also works well for the regime of deep ultra-strong coupling when $\lambda \geq \omega$ [21]. This adiabatic approximation generates an adiabatic potential with two sheets. The lower sheet has two minima if $\lambda \geq \sqrt{\omega\Delta}$ and only one minimum if $\lambda < \sqrt{\omega\Delta}$ [21]. When $\lambda \geq \sqrt{\omega\Delta}$ an approximate solution based on the displaced oscillators generated by the the adiabatic potential is given in Ref. [22]. However, the case of the adiabatic potential with just one minimum can be described by the Hamiltonian (5) of which both the eigenvalues [17] and the eigenvectors [20] are well reproduced by Eqs. (5)-(7). We note here that in the regime $\Delta \gg \omega$ a series expansion of $e^{\lambda S}$ gives rather similar results with Eq. (7). Moreover, one can easily check that the curvatures of the two adiabatic sheets in the origins are just ${\omega_-}^2$ and ${\omega_+}^2$, respectively. The eigenvector (7) exhibits also a certain degree of squeezing. In fact, the largest squeezing is encountered at $\lambda = \lambda_c = \sqrt{\omega\Delta}$ [23], where the system undergoes a sharp transition [24].

4. CONCLUSIONS

In this work we studied the Rabi Hamiltonian in the dispersive regime and ultra-strong coupling. It was used a unitary transformation that takes into account terms beyond the rotating wave approximation. We are able to build the approximate Hamiltonian with its energy levels and its eigenfunctions. It turns out that an exponential approximation of the eigenfunctions is better suited than the approximation made by series expansion. We also compare and discuss this approximation with respect to other approximations in the regimes of fast and slow two-level system.

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