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Adiabatic elimination of a nearly resonant quantum state

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Abstract
Quantum systems with multiple states are often reduced to simpler systems by adiabatic elimination of far-off-resonant states. This method provides accurate coupling and Stark shifts in the reduced system for very large values of the detunings only, far greater than that of the relevant couplings. We introduce two alternative techniques for exclusion of an off-resonant state based on the adiabatic and superadiabatic approximations, which provide far more accurate expressions for the coupling and the Stark shifts in the reduced system, and which are valid in much broader ranges of interaction parameters than the traditional adiabatic elimination method. The reason is that the conditions for the adiabatic and superadiabatic approximations only demand, for smooth pulse shapes, the detuning to be greater than the Fourier width of the pulse; hence, these approximations can be used even when the couplings exceed the detunings, i.e. when the excluded states can be described as 'nearly resonant'. The error of the adiabatic and superadiabatic approximations can be easily suppressed below the quantum computing benchmark of 10^{-4}, an objective that is hard to achieve with the traditional adiabatic elimination method.

(Some figures may appear in colour only in the online journal)

1. Introduction

Adiabatic elimination is a basic tool for reduction of complex quantum systems with multiple linkages to simpler effective systems with fewer linkages by removing weakly coupled states that are far off resonance with the relevant external fields. A few different (but related) approaches obtain the same reduced system wherein the properties of the adiabatically eliminated state are imprinted onto the effective couplings and the light (or ac Stark) shifts. These approaches include the second-order perturbation theory, formal integration of the Schrödinger equation with subsequent expansion of the ensuing integrals via integration by parts, mere annulling of the derivatives of the off-resonant states, and others [1, 2]. The validity of this approximation has been examined in great detail by several authors [3–6]. Regardless of the derivation, the condition for validity of the adiabatic elimination is that the detuning Δ in each transition is far greater than the Rabi frequency Ω of the respective driving field: $|\Delta| \gg \Omega$.

Recently, we have shown that the traditional adiabatic elimination, when applied to an off-resonant two-state system, can provide an accurate estimate for the acquired dynamic phase shift, with an error below the quantum computing benchmark of 10^{-4} [7], only for very large values of the detuning Δ [8]. We have proposed to use instead the adiabatic approximation, which is a far more accurate tool for evaluation of phase shifts, with a vast domain of validity: for smooth pulse shapes, it demands simply $\Delta \gtrsim 1/T$, where T is the pulse width [9]. The accuracy is further enhanced by superadiabatic corrections [8]. We can therefore claim that this approach is applicable from far-off-resonant to *nearly resonant* states equally well.

In this work we extend this approach to the elimination of off-resonant states in quantum systems with multiple states, with special attention given to the elimination of the middle state in three-state chainwise connected systems. Two important examples of three-state chains are the ladder and Λ systems. Ladder systems are found in resonantly enhanced

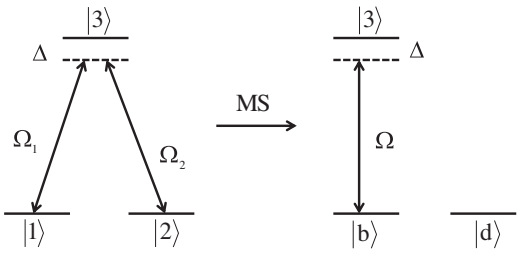

Figure 1. Linkage diagram for a three-state lambda system (left), and the same system after Morris–Shore transformation (right). Ω_1 and Ω_2 are the Rabi frequencies and Δ is the detuning.

two-photon excitation in many atoms, for instance, in the 5s–5p–5d transition chain in rubidium wherein state 5p is nearly midway between states 5s and 5d [10]. Typical Λ systems are the Raman transitions between two ground states via an excited state. Raman transitions are a very popular tool for qubit manipulations in quantum information processing [7] because they allow the qubit to be formed of ground states; for example, the so-called radio-frequency qubits possess much longer coherence times than the optical qubits [11].

2. Model system

Because in the present context the ladder and Λ systems are treated identically, we shall only consider a three-state quantum system in a Λ configuration, interacting with two coherent fields as illustrated in figure 1(left); the results extend to ladder systems in an obvious manner. We wish to estimate the transition probability from state $|1\rangle$ to state $|2\rangle$ when the middle state $|3\rangle$ is off-single-photon resonance by a detuning Δ. The evolution of the system is described by the time-dependent Schrödinger equation:

$$\mathrm{i}\hbar\partial_t \mathbf{c}(t) = \mathbf{H}(t)\mathbf{c}(t), \tag{1}$$

where $\mathbf{c}(t)$ is the vector column with the probability amplitudes and the Hamiltonian of the system, after setting the standard rotating wave approximation [1, 2], is

$$\mathbf{H}(t) = \frac{\hbar}{2}\begin{bmatrix} 0 & 0 & \Omega_1(t) \\ 0 & 0 & \Omega_2(t) \\ \Omega_1(t)^* & \Omega_2(t)^* & 2\Delta \end{bmatrix}, \tag{2}$$

where $\Omega_1(t)$ is the Rabi frequency of the coupling between states $|1\rangle$ and $|3\rangle$ and $\Omega_2(t)$ is the Rabi frequency of the coupling between states $|2\rangle$ and $|3\rangle$. Each Rabi frequency parameterizes the coupling between the corresponding driving electric field with an envelope $\mathbf{E}(t)$ and the relevant transition dipole moment $\mathbf{d}$: $\Omega(t) = -\mathbf{d}\cdot\mathbf{E}(t)/\hbar$. Here, $\Delta = \omega_1^0 - \omega_1 = \omega_2^0 - \omega_2$ is the one-photon detuning between the laser carrier frequencies ω_j and the Bohr transition frequencies ω_j^0, with $j = 1, 2$. For simplicity, we assume hereafter that the detuning is constant, $\Delta = \text{const}$. We also assume that the first and last states of the chain are on two-photon resonance, as evident from the zeros in the first two diagonal elements.

3. Adiabatic elimination

The traditional adiabatic elimination is applicable when the detuning Δ is very large,

$$|\Delta| \gg \Omega(t), \tag{3}$$

where $\Omega(t) = \sqrt{|\Omega_1(t)|^2 + |\Omega_2(t)|^2}$ is the root-mean-square (RMS) Rabi frequency. In this limit, the population of state $|3\rangle$ is strongly suppressed, $P_3(t) \sim \Omega(t)^2/\Delta^2 \ll 1$. The easiest route to adiabatic elimination of state $|3\rangle$ is to set $\partial_t c_3(t) = 0$ and replace the ensuing expression for $c_3(t)$ in the other two equations. State $|3\rangle$ is thereby removed and we are left with an effective two-state system of states $|1\rangle$ and $|2\rangle$, described by the reduced Hamiltonian

$$\mathbf{H}^{\mathrm{e}}(t) = \frac{\hbar}{2}\begin{bmatrix} S_1^{\mathrm{e}}(t) & \Omega^{\mathrm{e}}(t) \\ \Omega^{\mathrm{e}}(t)^* & S_2^{\mathrm{e}}(t) \end{bmatrix}, \tag{4}$$

where

$$\Omega^{\mathrm{e}}(t) = -\frac{\Omega_1(t)\Omega_2(t)^*}{2\Delta}, \tag{5a}$$

$$S_k^{\mathrm{e}}(t) = -\frac{|\Omega_k(t)|^2}{2\Delta} \quad (k = 1, 2). \tag{5b}$$

These are the well-known expressions for the two-photon coupling and the Stark shifts resulting from the adiabatic elimination of state $|3\rangle$; the latter is often called a 'virtual' state. The vast popularity of this method is routed in the extreme simplicity of the reduced Hamiltonian. However, it is only applicable when condition (3) is fulfilled, which guarantees that the population $P_3(t)$ remains negligibly small at all times: $P_3(t) \ll 1$.

4. Adiabatic approximation

We introduce now an alternative approach based upon the adiabatic approximation, which does not necessarily require $P_3(t) \ll 1$. In fact, the population $P_3(t)$ may reach significant transient values during adiabatic evolution but it returns to zero in the end due to the effect of adiabatic population return [12]. Consequently, this approach allows us to calculate the effective coupling between states $|1\rangle$ and $|2\rangle$ and the Stark shifts for a much wider range of parameter values than condition (3).

We start again from the Hamiltonian (2). We assume that $\Omega_1(t)$ and $\Omega_2(t)$ share the same time dependence[3]

$$\Omega_1(t) = \beta_1 f(t), \quad \Omega_2(t) = \beta_2 f(t), \tag{6}$$

and hence, $\Omega(t) = \beta f(t)$, where $\beta = \sqrt{|\beta_1|^2 + |\beta_2|^2}$. We apply the Morris–Shore (MS) transformation [13], which decomposes the initial system into a decoupled (dark) state $|d\rangle$ and a two-state system composed of a bright ground state $|b\rangle$ and the original state $|3\rangle$, as shown in figure 1, where [14]

$$|d\rangle = \frac{\beta_2}{\beta}|1\rangle - \frac{\beta_1}{\beta}|2\rangle, \tag{7a}$$

$$|b\rangle = \frac{\beta_1^*}{\beta}|1\rangle + \frac{\beta_2^*}{\beta}|2\rangle. \tag{7b}$$

[3] The condition for the same time dependence of the Rabi frequencies is not mandatory for the application of our method.

The (constant) transformation matrix reads

$$\mathbf{B} = \begin{bmatrix} \beta_2^*/\beta & \beta_1/\beta & 0 \\ -\beta_1^*/\beta & \beta_2/\beta & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{8}$$

and the transformed Hamiltonian in the MS basis is

$$\mathbf{H}_{\rm MS}(t) = \mathbf{B}^\dagger \mathbf{H}(t)\mathbf{B} = \frac{\hbar}{2}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \Omega(t) \\ 0 & \Omega(t) & 2\Delta \end{bmatrix}. \tag{9}$$

Next we make a transformation to the adiabatic basis, i.e. the basis of eigenstates of $\mathbf{H}_{\rm MS}(t)$: $\{|d\rangle, |a_1\rangle, |a_2\rangle\}$, with

$$|a_1\rangle = \cos\theta(t)|b\rangle - \sin\theta(t)|3\rangle, \tag{10a}$$

$$|a_2\rangle = \sin\theta(t)|b\rangle + \cos\theta(t)|3\rangle, \tag{10b}$$

where

$$\theta(t) = \tfrac{1}{2}\arctan[\Omega(t)/\Delta]. \tag{11}$$

Explicitly, the transformation matrix reads

$$\mathbf{A}(t) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta(t) & \sin\theta(t) \\ 0 & -\sin\theta(t) & \cos\theta(t) \end{bmatrix}, \tag{12}$$

and the Hamiltonian in the adiabatic MS basis is $\widetilde{\mathbf{H}}_{\rm MS}(t) = \mathbf{A}(t)^\dagger \mathbf{H}_{\rm MS}\mathbf{A}(t) - \mathrm{i}\hbar\mathbf{A}(t)^\dagger\partial_t\mathbf{A}(t)$; explicitly,

$$\widetilde{\mathbf{H}}_{\rm MS}(t) = \frac{\hbar}{2}\begin{bmatrix} 0 & 0 & 0 \\ 0 & \Delta - \lambda(t) & -2\mathrm{i}\partial_t\theta(t) \\ 0 & 2\mathrm{i}\partial_t\theta(t) & \Delta + \lambda(t) \end{bmatrix}, \tag{13}$$

where

$$\lambda(t) = \sqrt{\Delta^2 + \Omega(t)^2}. \tag{14}$$

If the evolution is adiabatic, then we can neglect the off-diagonal elements $\pm\mathrm{i}\partial_t\theta(t)$ in equation (13). We find thereby the *adiabatic approximation* $\widetilde{\mathbf{H}}^{\rm a}_{\rm MS}(t)$ to the Hamiltonian $\widetilde{\mathbf{H}}_{\rm MS}(t)$ in the adiabatic MS basis,

$$\widetilde{\mathbf{H}}^{\rm a}_{\rm MS}(t) = \frac{\hbar}{2}\begin{bmatrix} 0 & 0 & 0 \\ 0 & \Delta - \lambda(t) & 0 \\ 0 & 0 & \Delta + \lambda(t) \end{bmatrix}. \tag{15}$$

Next we roll back the MS transformation $\mathbf{B}$ to a basis of three new states $|\widetilde{1}\rangle$, $|\widetilde{2}\rangle$ and $|\widetilde{3}\rangle$; the Hamiltonian in this basis reads $\mathbf{H}^{\rm a}(t) = \mathbf{B}\widetilde{\mathbf{H}}^{\rm a}_{\rm MS}(t)\mathbf{B}^\dagger$. These states are obtained from states $|1\rangle$, $|2\rangle$ and $|3\rangle$ after successively making the transformations $\mathbf{B}$, $\mathbf{A}$ and $\mathbf{B}^\dagger$; explicitly, they read

$$|\widetilde{1}\rangle = \frac{|\beta_1|^2\cos\theta + |\beta_2|^2}{\beta^2}|1\rangle + \frac{\beta_1\beta_2^*(\cos\theta - 1)}{\beta^2}|2\rangle - \frac{\beta_1}{\beta}\sin\theta|3\rangle, \tag{16a}$$

$$|\widetilde{2}\rangle = \frac{\beta_1^*\beta_2(\cos\theta - 1)}{\beta^2}|1\rangle + \frac{|\beta_1|^2 + |\beta_2|^2\cos\theta}{\beta^2}|2\rangle - \frac{\beta_2}{\beta}\sin\theta|3\rangle, \tag{16b}$$

$$|\widetilde{3}\rangle = \frac{\beta_1^*}{\beta}\sin\theta|1\rangle + \frac{\beta_2^*}{\beta}\sin\theta|2\rangle + \cos\theta|3\rangle. \tag{16c}$$

State $|\widetilde{3}\rangle$ is the one which is eliminated, since in the adiabatic limit it is decoupled from states $|\widetilde{1}\rangle$ and $|\widetilde{2}\rangle$, which can be seen if we write the Hamiltonian in this basis. Furthermore, states $|\widetilde{1}\rangle$, $|\widetilde{2}\rangle$ and $|\widetilde{3}\rangle$ have the asymptotics[4]

$$\lim_{t\to\pm\infty}|\widetilde{1}\rangle = |1\rangle, \tag{17a}$$

$$\lim_{t\to\pm\infty}|\widetilde{2}\rangle = |2\rangle, \tag{17b}$$

$$\lim_{t\to\pm\infty}|\widetilde{3}\rangle = |3\rangle, \tag{17c}$$

which means that for adiabatic evolution the population in state $|\widetilde{3}\rangle$ remains zero. Hence, the reduced basis involves states $|\widetilde{1}\rangle$ and $|\widetilde{2}\rangle$ only. Our method therefore allows us to calculate the transition probability from state $|1\rangle$ to state $|2\rangle$, even though we are using the basis of states $|\widetilde{1}\rangle$ and $|\widetilde{2}\rangle$, because, owing to equations (17), the probability of the transition $|1\rangle \to |2\rangle$ is equal to the probability of the transition $|\widetilde{1}\rangle \to |\widetilde{2}\rangle$. By the same token, the propagators in the bases $\{|\widetilde{1}\rangle, |\widetilde{2}\rangle, |\widetilde{3}\rangle\}$ and $\{|1\rangle, |2\rangle, |3\rangle\}$ are equal too. It is easy to verify that in the limit (3), relations (17) are fulfilled at any time, not only asymptotically at $t \to \pm\infty$.

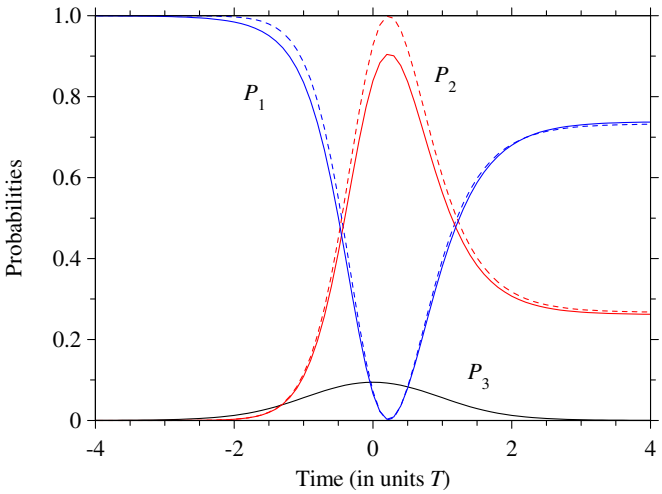

Figure 2. Time evolution of the exact probabilities (solid lines), compared with those, calculated by using the adiabatic approximation (dashed lines), for hyperbolic secant pulse shape with $\beta = 10/T$ and $\Delta = 8/T$.

In the original basis we can have a transient population in state $|3\rangle$, while state $|\widetilde{3}\rangle$ remains decoupled and its population is zero during the entire evolution. This feature is illustrated in figure 2, where we compare the time evolution of the populations of states $|1\rangle$, $|2\rangle$ and $|3\rangle$ with the ones for states $|\widetilde{1}\rangle$ and $|\widetilde{2}\rangle$.

Explicitly, the Hamiltonian driving the adiabatically reduced system of states $|\widetilde{1}\rangle$ and $|\widetilde{2}\rangle$ reads

$$\mathbf{H}^{\rm a}(t) = \frac{\hbar}{2}\begin{bmatrix} S_1^{\rm a}(t) & \Omega^{\rm a}(t) \\ \Omega^{\rm a}(t)^* & S_2^{\rm a}(t) \end{bmatrix}, \tag{18}$$

where

$$\Omega^{\rm a}(t) = \frac{\beta_1\beta_2^*}{\beta^2}\Delta\left[1 - \sqrt{1 + \frac{\Omega(t)^2}{\Delta^2}}\right], \tag{19a}$$

[4] The limits of $t \to \pm\infty$ are only meaningful if the fields are pulse shaped. Otherwise, our technique can still be applied by changing the limits to any finite t_i and t_f.

$$S_k^{\rm a}(t) = \frac{|\beta_k|^2}{\beta^2}\Delta\left[1-\sqrt{1+\frac{\Omega(t)^2}{\Delta^2}}\right] \quad (k=1,2). \qquad (19b)$$

For large Δ, equation (3), we have

$$\Delta\left[1-\sqrt{1+\frac{\Omega(t)^2}{\Delta^2}}\right] = -\frac{\Omega(t)^2}{2\Delta}+\frac{\Omega(t)^4}{8\Delta^3}+\mathcal{O}(\Delta^{-5}), \qquad (20)$$

and the coupling and the shifts of equations (19) reduce to the corresponding coupling and shifts of equations (5) obtained by the standard adiabatic elimination. The third term in equation (20), which gives the lowest order correction to equations (5), confirms condition (3) for the validity of expressions (5) for the coupling and the Stark shift in the adiabatic elimination approximation.

5. Adiabatic condition

We neglected the non-adiabatic terms $\pm i\partial_t\theta(t)$ in equation (13) with the assumption of adiabatic evolution. Thorough analysis of the adiabatic condition has been conducted by various authors [9, 12, 15, 16]. In general, the non-adiabatic coupling $|\partial_t\theta(t)|$ must be small compared to the eigenenergy splitting $\lambda(t)$; for constant detuning, as assumed here, we find

$$\frac{|\Delta\partial_t\Omega(t)|}{\Omega(t)^2+\Delta^2} \ll \sqrt{\Omega(t)^2+\Delta^2}. \qquad (21)$$

Because we assume that the original system of states $\{|1\rangle, |2\rangle, |3\rangle\}$ is initially in state $|1\rangle$ or state $|2\rangle$, or in a superposition of them, this implies that the MS system $\{|d\rangle, |b\rangle, |3\rangle\}$ is initially in state $|d\rangle$ or state $|b\rangle$, or in a superposition of them. The dark state $|d\rangle$ is unaffected regardless of the interaction. When the adiabatic condition (21) is satisfied the population in the MS two-state system $|b\rangle \leftrightarrow |3\rangle$, after a temporary partial excursion to state $|3\rangle$, undergoes *complete population return* to the initial state $|b\rangle$ [12], because the detuning is constant. The absence of population change in the MS basis, however, does not mean the same in the original basis of states $|1\rangle, |2\rangle, |3\rangle$: there, the population may be redistributed between states $|1\rangle$ and $|2\rangle$.

For two of the most important pulse shapes, hyperbolic secant, $f(t) = \mathrm{sech}(t/T)$, and Gaussian, $f(t) = \exp(-t^2/T^2)$, the adiabatic condition demands, respectively,

$$\frac{\ln(4/\epsilon)}{\pi T} < |\Delta|, \qquad (22a)$$

$$\beta < 0.76|\Delta|\exp\left[\frac{\pi^2\Delta^2T^2}{4\ln^2(4/\epsilon)}-\frac{\ln^2(4/\epsilon)}{4\Delta^2T^2}\right]. \qquad (22b)$$

These conditions are derived from the exact formula for the transition probability of the Rosen–Zener model for a sech pulse [17], and from a highly accurate approximate formula for a Gaussian pulse [9]. These conditions set relations for which the post-pulse transition probability of the eliminated state $|3\rangle$ is $P_3 < \epsilon \ll 1$; they are illustrated in figure 3 for $\epsilon = 0.01$.

A crucial observation from the adiabatic conditions (22) and figure 3 is that for these smooth pulse shapes, the adiabatic regime is reached when the detuning exceeds just a few spectral pulse widths $1/T$: just about $2/T$ for the sech pulse shape and a little larger values for the Gaussian pulse shape, which is less adiabatic because of its steeper rising and falling edges. Obviously, for sech pulses the adiabatic condition does not depend at all on the Rabi frequency, while for Gaussian pulses there is a weak logarithmic dependence on the Rabi frequency. The ensuing physical implication—the absent, or very weak, power broadening—has been observed experimentally [12]. An important consequence from here is that adiabatic evolution can be achieved even when the Rabi frequency exceeds greatly the detuning, as seen in figure 3. Then the adiabatic elimination, which demands condition (3), is completely inadequate, but the adiabatic approximation is perfectly applicable. This remarkable feature explains why the parameter ranges for the adiabatic approximation are much broader than those for the adiabatic elimination.

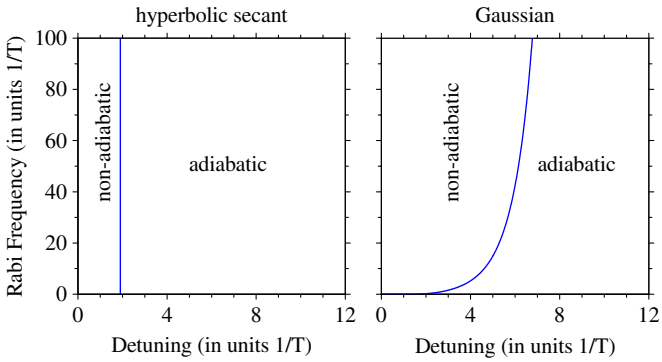

Figure 3. Adiabatic condition for the hyperbolic secant pulse, equation (22*a*) (left), and Gaussian pulse, equation (22*b*) (right), as a function of the detuning Δ and the RMS peak Rabi frequency β. On the right of the dividing lines the final population of the eliminated state $|3\rangle$ $P_3 < 0.01$ and hence the evolution can be assumed adiabatic within this deviation.

6. Superadiabatic approximation

The adiabatic approximation evaluates very accurately the transition probability in the reduced two-state system, as we shall see below. However, even greater accuracy can be achieved if we continue the diagonalization procedure to the first superadiabatic basis. For this purpose, we diagonalize the Hamiltonian (13) and obtain the superadiabatic Hamiltonian, which has a similar structure as equation (13). Next we neglect the superadiabatic coupling, roll back the transformation **B** and find the effective coupling and the Stark shifts

$$\Omega^{\rm s}(t) = \frac{\beta_1\beta_2^*}{\beta^2}\Delta\left[1-\sqrt{1+\frac{\Omega(t)^2+4(\partial_t\theta(t))^2}{\Delta^2}}\right], \qquad (23a)$$

$$S_k^{\rm s}(t) = \frac{|\beta_k|^2}{\beta^2}\Delta\left[1-\sqrt{1+\frac{\Omega(t)^2+4(\partial_t\theta(t))^2}{\Delta^2}}\right], \qquad (23b)$$

with $k = 1, 2$. Obviously, the difference between the superadiabatic approximation (23) and the adiabatic approximation (19) is in the non-adiabatic terms with $(\partial_t\theta(t))^2$. One can continue and derive higher order superadiabatic corrections, which further improve the

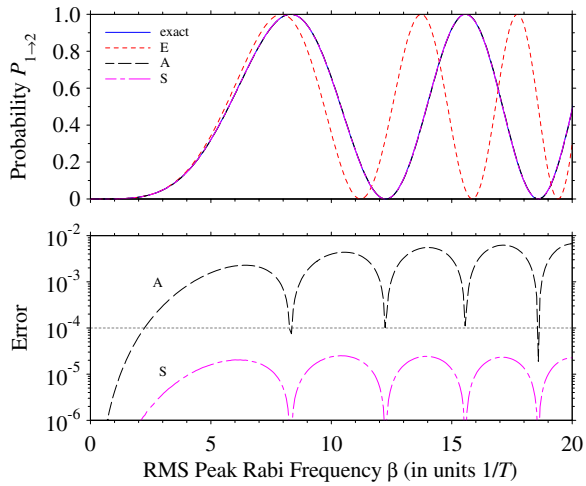

Figure 4. Transition probability $P_{1\to2}$ versus RMS peak Rabi frequency β for a hyperbolic secant pulse shape with $\beta_1 = \beta_2 = \beta/\sqrt{2}$ and $\Delta = 10/T$. The exact probability, calculated by solving numerically the Schrödinger equation for the original three-state system, is compared with the transition probabilities in the reduced two-state systems derived from the adiabatic elimination (curve E, equations (5)), the adiabatic approximation (curve A, equations (19)) and the superadiabatic approximation (curve S, equations (23)). In the top frame, the curves A and S are indiscernible from the exact curve; for this reason, their accuracy is examined in the bottom frame.

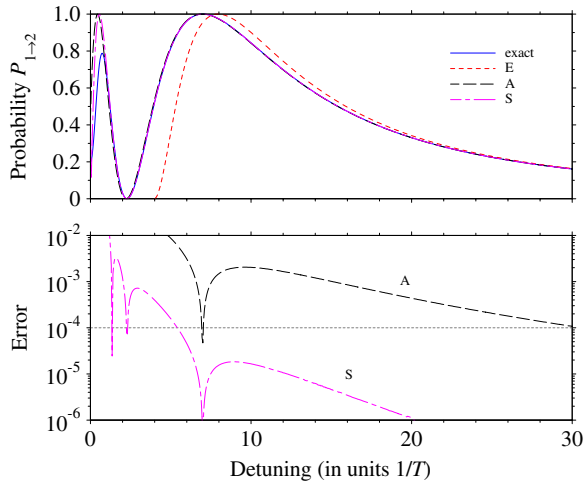

Figure 5. The same as shown in figure 4 but the transition probability $P_{1\to2}$ is plotted versus the detuning Δ for peak Rabi frequencies $\beta_1 = \beta_2 = 5/T$ (hence $\beta = 5\sqrt{2}/T$).

accuracy; however, we have concluded that the superadiabatic approximation (23) suffices to evaluate the dynamics in the reduced two-state system with an accuracy exceeding the quantum computing benchmark.

7. Examples

Figures 4 and 5 compare the exact post-pulse population of state $|2\rangle$, calculated by solving numerically the Schrödinger equation (1) with the Hamiltonian (2), with the approximations derived from the adiabatic elimination, the adiabatic approximation and the superadiabatic approximation. In

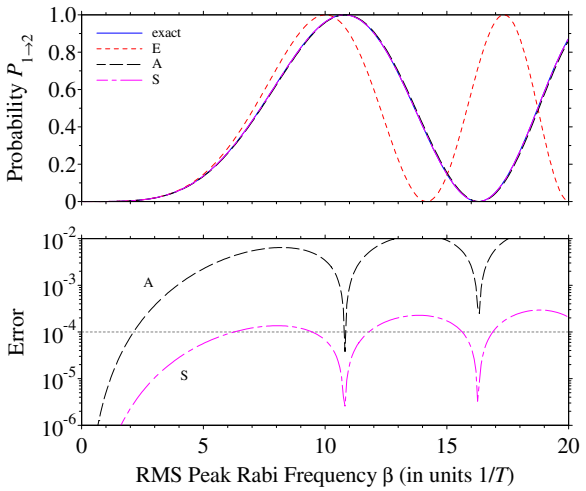

Figure 6. Same as shown in figure 4, but for a Gaussian pulse shape.

figure 4, which shows the post-pulse population of state $|2\rangle$ versus the RMS Rabi frequency β, the traditional adiabatic elimination fails already when β approaches $\Delta/2$ and it is completely inadequate beyond this value. The adiabatic and superadiabatic approximations remain highly accurate even when the RMS Rabi frequency exceeds the detuning considerably and are indiscernible from the exact curve in the upper frame of figure 4. The lower frame shows the errors of these approximations, which remain well below 10^{-2} for the adiabatic approximation, and well below the quantum computing benchmark 10^{-4} for the superadiabatic approximation.

Similar conclusions are derived from figure 5 where the post-pulse population of state $|2\rangle$ is plotted versus the detuning Δ. The adiabatic elimination curve approaches the exact values for $|\Delta| \gg \beta$ only, while the error of the adiabatic approximation decreases rapidly as Δ grows. The error of the superadiabatic approximation falls below the 10^{-4} benchmark already for $\Delta \sim \beta$. Clearly, the adiabatic and superadiabatic approximations fail only in the limit $\Delta \to 0$, as expected. These features are in complete agreement with the adiabatic condition (22*a*) illustrated in figure 3.

In figure 6, we plot the post-pulse transition probability as a function of the RMS Rabi frequency for Gaussian pulse shapes. The fact that Gaussian pulses are less adiabatic than the hyperbolic secant leads to lower accuracy. However, an accuracy of 10^{-4} can still be accomplished using the superadiabatic approximation.

8. Conclusions

The widely used technique of adiabatic elimination of off-resonant states in quantum systems provides the correct couplings and light shifts in the reduced system for very large values of the detuning only, $|\Delta| \gg \Omega(t)$. We have introduced two alternative techniques for exclusion of an off-resonant state based upon the adiabatic and superadiabatic approximations; for large detuning, these reduce to the expressions obtained by the adiabatic elimination method. However, because the conditions for adiabatic evolution

impose much weaker restrictions on the interaction parameters than the adiabatic elimination condition, the resulting coupling and light shifts in the adiabatic and superadiabatic approximations are valid in much broader ranges of interaction parameters. The superadiabatic approximation, in particular, allows us to easily suppress the error below the quantum computing benchmark of 10^{-4}; this is possible also with the adiabatic approximation albeit in a more restricted parameter domain. For smooth pulse shapes, the condition for the adiabatic and superadiabatic approximations is merely $|\Delta| \gtrsim 1/T$, with only weak dependence on the Rabi frequency possible. Therefore, these approximations can be used for $\Omega \gg |\Delta|$, a domain where the adiabatic elimination is completely inadequate; hence, we can claim that in this manner we can eliminate 'nearly resonant' states.

Finally, we point out that we have focused our attention to three-state chainwise connected systems. However, the methods for exclusion of off-resonant states introduced here are applicable to arbitrary quantum systems with discrete energy states by selecting an appropriate subspace and carrying out the exclusion routine over this subspace.

Acknowledgments

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