Level splitting in association with the multiphoton Bloch–Siegert shift

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Abstract
We present a unitary equivalent spin-boson Hamiltonian in which terms can be identified which contribute to the Bloch–Siegert shift, and to the level splittings at the anticrossings associated with the Bloch–Siegert resonances. First-order degenerate perturbation theory is used to develop approximate results in the case of moderate coupling for the level splitting.

1. Introduction
The dynamics of a two-level with sinusoidal coupling has been of interest since the time of Bloch and Siegert [1, 2]. The (closely related) basic model for a two-level system coupled to a simple harmonic oscillator was considered by Cohen-Tannoudji et al [3]. The coupling in these models produces an increase in the two-level system transition energy (sometimes termed the Bloch–Siegert shift). As the coupling strength is increased, the levels shift relative to one another, producing both level crossings and level anticrossings. Level crossings occur when the dressed two-level transition energy matches an even number of oscillator quanta (in which case the parity of the states is mismatched, so no mixing occurs). Level anticrossings occur when the dressed two-level transition energy is resonant with an odd number of oscillator quanta, with the magnitude of the splitting indicative of the ability of the coupled system to convert energy between the two different degrees of freedom.

These models were studied initially in the context of spin dynamics in a magnetic field [1, 2], but they also appear in other applications. The coupling between atoms and an electromagnetic field can in some cases be described by these models, in which case the resonances mentioned above correspond to multiphoton interactions. Multiphoton resonances in which a substantial number of photons are exchanged have become experimentally accessible recently [4]. In part because of this there has been renewed interest in the multiphoton regime [5, 6]. One need keep in mind that in a real multi-level system the two-level approximation itself may break down, under conditions where the coupling becomes very strong between two levels.

2. Unitary equivalent Hamiltonian
The Hamiltonian for the coupled two-level system and oscillator of interest (the spin-boson Hamiltonian) can be written as

\[ \hat{H} = \frac{\Delta E}{2} \hat{\sigma}_z + \hbar \omega_0 \hat{a} \hat{a}^\dagger + U (\hat{a}^\dagger + \hat{a}) \hat{\sigma}_x \]  

where \( \hat{\sigma}_i \) are the Pauli matrices and \( U \) is the linear coupling constant between the oscillator and the two-level system. Since we are interested in the multiphoton regime, we assume that the background excitation of the photon field is large:

\[ \Delta E \gg \hbar \omega_0, \quad n \gg 1. \]  

Rotations are often used to simplify Hamiltonians [7]; however, in this case our rotation will make the problem more complicated mathematically but perhaps simpler functionally as outlined above. We consider the unitary equivalent Hamiltonian

\[ \hat{H}' = \hat{U}^\dagger \hat{H} \hat{U} \]  

The condition for Bloch–Siegert resonances can be written as

$$\Delta E(g) = (2k + 1)\hbar\omega_0. \quad (13)$$

Level crossings occur in the modified version of the problem described by the unperturbed Hamiltonian $\hat{H}_0$ in the rotated frame. As level anticrossing occur in the original spin-boson model at these resonances, the coupling that is responsible for the level anticrossing has been eliminated in $\hat{H}_0$. This is an interesting and perhaps unexpected feature of this rotation.

4. Level splitting in the unrotated Hamiltonian

Near a resonance, we can use a two-level description to account for the level splittings:

$$E(g) \left( c_0 \atop c_1 \right) = \left( E_0(g) \atop v \atop E_1(g) \right) \left( c_0 \atop c_1 \right). \quad (14)$$

Two levels with energies $E_0$ and $E_1$ that depend on the dimensionless coupling strength $g$, cross, and couple to each other with an interaction $v$ which we assume to be constant in the vicinity of the resonance. At resonance ($g_0$), the two levels in this simplified model are degenerate

$$E_0(g_0) = E_1(g_0). \quad (15)$$

The splitting between the two levels at this point is twice the magnitude of the interaction

$$\Delta E_{\text{min}} = E_+(g_0) - E_-(g_0) = 2|v|. \quad (16)$$

The level splittings in the case of weak coupling have been known for some time [2], as mentioned above. Shirley’s results written in our notation are

$$\Delta E_{\text{min}} = \frac{g_{0}^{2}}{2k} \left( \frac{\Delta E}{\hbar \omega_0} \right)^{2k} \Delta E. \quad (17)$$

We have plotted results from the direct numerical solution of the spin-boson Hamiltonian (equation (1)), and also for the weak coupling result in figure 1. When the dimensionless coupling constant $g$ is small the results match well; when the coupling gets stronger, we see (as expected) that perturbation theory begins to break down.

5. Level splitting in the rotated Hamiltonian

The dressed transition energy of the two-level system is described reasonably well through the unperturbed part $\hat{H}_0$ of the rotated Hamiltonian, but no level splittings occur in the eigenvalues of $\hat{H}_0$. Hence, all of the splitting must be due
to the terms we have considered to be perturbations. In this section, our goal is to apply degenerate perturbation theory in the rotated frame to see whether the larger of the perturbation terms $\hat{V}$ can account for the level splitting.

To calculate the level splitting in the vicinity of an anticrossing, we need to compute the eigenfunctions $\psi_{n,m}$ of $\hat{H}_0$ where

$$\hat{H}_0 \psi_{n,m} = E_{n,m} \psi_{n,m}. \quad (18)$$

This can be done numerically, or by using the WKB approximation (which we have found to be effective for such problems). Near the $(2k+1)$th resonance, the level anticrossing is well described by a simple two-level approximation

$$E(g) \begin{pmatrix} \zeta_0 \\ \zeta_1 \end{pmatrix} = \begin{bmatrix} E_{n,m}(g) & \langle \psi_{n,m} | \hat{V} | \psi_{n+2k+1,m-1} \rangle \\ \langle \psi_{n+2k+1,m-1} | \hat{V} | \psi_{n,m} \rangle & E_{n+2k+1,m-1}(g) \end{bmatrix} \begin{pmatrix} \zeta_0 \\ \zeta_1 \end{pmatrix}. \quad (19)$$

The energy splitting at resonance is

$$\Delta E_{\text{min}} = E_+ (g_0) - E_- (g_0) = 2 |\langle \psi_{n,m} | \hat{V} | \psi_{n+2k+1,m-1} \rangle|. \quad (20)$$

In figure 2, we have plotted level splittings taken from a direct numerical solution of the original spin-boson Hamiltonian (equation (1)) and also from first-order degenerate perturbation theory as discussed here (we used numerical solutions for the eigenfunctions $\psi_{n,m}$ for this result). We can see from figure 2 that the exact numerical results for the level splitting of the unrotated Hamiltonian match very well the results obtained by using degenerate perturbation theory on the rotated Hamiltonian. Minor deviations occur at the larger $g$ values which we attribute to the omission of higher-order terms in the degenerate perturbation theory.

6. Conclusion

We have found a useful unitary transformation that produces a rotated Hamiltonian for the spin-boson problem in the multiphoton regime that has interesting properties. The rotated Hamiltonian is more complicated mathematically than the initial spin-boson Hamiltonian, but appears to be simpler in terms of functionality. One part of the rotated Hamiltonian is identified as an unperturbed Hamiltonian ($\hat{H}_0$) which appears to describe the coupled systems reasonably well away from the level anticrossings. This part of the problem is useful for developing estimates of the Bloch–Siegert shift. Another part of the rotated Hamiltonian ($\hat{V}$) is identified as a perturbation which is responsible for most of the coupling which occurs at the anti-crossing. Used with first-order degenerate perturbation theory, this term provides a reasonable approximation for the level splittings at the Bloch–Siegert resonances. Finally, there is present an additional term ($\hat{W}$) in the rotated Hamiltonian which is small (so that we have neglected it in our discussion here), but which can provide a minor correction to the dressed two-level system energies.

Note that the approach used in this paper can be applied to other problems as well. We have used a similar unitary transformation on the spin-1 version of the problem, in which case a similar rotated Hamiltonian is obtained [10]. In this more complicated situation, we again obtain a similar unperturbed Hamiltonian which gives a good approximation for the coupled system away from the level anticrossings, and a similar perturbation which accounts for most of the level splittings at the Bloch–Siegert resonances. From this perspective, the two problems seem to be quite similar. However, the spin-1 problem exhibits additional complexity not found in the simpler spin-boson problem. It is possible in the spin-1 problem for the coupled system to be sufficiently perturbed by the resonant exchange of one quantum of two-level system energy that a second cannot be transferred. This is the case when the oscillator excitation is sufficiently low that
the addition of a dressed two-level system transition energy results in a minor increase in the Bloch–Siegert shift, which spoils the resonance condition.

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Appendix. WKB approximations
In this appendix, we are interested in the development of WKB (or JWKB) approximations for energy levels and matrix elements. We begin with the time-independent Schrödinger equation for the separated and rotated $\hat{H}_0$ problem (equation (9)) rewritten as

$$\epsilon \psi(y) = -\frac{d^2}{dy^2}\psi(y) + v(y)\psi(y) \quad (A.1)$$

where

$$\epsilon = \frac{2E}{\hbar\omega_0} + 1, \quad v(y) = y^2 + \frac{2m}{\hbar\omega_0}\Delta E^2 + 8U^2 y^2.$$  

A.1. Approximate WKB solution
A WKB solution is developed according to [9]

$$\psi(y) = \frac{\sin \phi(y)}{\sqrt{n(y)}} \quad (A.2)$$

where the phase $\phi(y)$ is related to $n(y)$ according to

$$\phi(y) = \int_{y_0}^{y} n(y') \, dy'.$$  

Within the WKB approximation in the allowed region, we approximate $n(y)$ by

$$n(y) = \sqrt{\epsilon - v(y)}.$$  

A.2. WKB eigenvalue equation
It is possible to develop quite an accurate estimate for the energy eigenvalue in the limit that $n$ is large by requiring the total phase within the allowed region to be an integral number of $\pi$ minus an appropriate offset. We may write

$$\phi(y_{\text{max}}) - \phi(y_{\text{min}}) = \int_{y_{\text{min}}}^{y_{\text{max}}} n(y') \, dy' = \left( n + \frac{1}{2} \right) \pi \quad (A.5)$$

where $y_{\text{min}}$ and $y_{\text{max}}$ are the classical turning points. The offset in this case has been selected to give exact agreement in the case of the simple harmonic oscillator potential. This equation is solved implicitly for the energy eigenvalue $\epsilon$, which can be done simply numerically using binary section or Newton’s method. We have found that for large $n$ the results are in excellent agreement with those obtained by direct numerical solution of the Schrödinger equation.

A.3. WKB estimate for the dressed energy $\Delta E(g)$
We found that a simple approximation to the energy eigenvalues can be obtained by adopting simple harmonic oscillator wavefunctions, in which case a variational energy estimate produces [11]

$$E_{n,m}(g) = \hbar \omega_0 (n|\hat{a}^\dagger \hat{a}|n) + (n|\sqrt{\Delta E^2 + 8U^2 y^2}|n)m. \quad (A.6)$$

The first term on the RHS simplifies to $n\hbar\omega_0$ since we are using simple harmonic oscillator wavefunctions. The second term on the RHS is more difficult to evaluate since the relevant integrals appear not to be available in closed form. Hence, we seek a WKB approximation.

In the WKB approximation, we may write

$$\langle n|\sqrt{\Delta E^2 + 8U^2 y^2}|n \rangle = \int_{y_{\text{min}}}^{y_{\text{max}}} \sqrt{\Delta E^2 + 8U^2 y^2} \, n(y') \, dy'.$$  

(A.7)

In the large-$n$ limit, the rapidly oscillating phases average out to a constant (1/2), and we may write

$$\langle n|\sqrt{\Delta E^2 + 8U^2 y^2}|n \rangle = \int_{y_{\text{min}}}^{y_{\text{max}}} \frac{\sqrt{\Delta E^2 + 8U^2 y^2}}{\sqrt{\epsilon - y^2}} \, dy'. \quad (A.8)$$

Since here we are using the WKB approximation for simple harmonic oscillator wavefunctions, we may write

$$n(y) = \sqrt{\epsilon - y^2} \quad y_{\text{min}} = -\sqrt{\epsilon} \quad y_{\text{max}} = \sqrt{\epsilon}$$

with $\epsilon = 2n + 1$; and

$$\int_{y_{\text{min}}}^{y_{\text{max}}} \frac{1}{n(y')} \, dy' = \pi. \quad (A.9)$$

Using this, we obtain

$$\langle n|\sqrt{\Delta E^2 + 8U^2 y^2}|n \rangle = \frac{1}{\pi} \int_{-\sqrt{\epsilon}}^{\sqrt{\epsilon}} \frac{\sqrt{\Delta E^2 + 8U^2 y^2}}{\sqrt{\epsilon - y^2}} \, dy$$

$$= \Delta E(g) \quad (A.10)$$

which is in agreement with equation (11).

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