Two-level systems coupled to oscillators

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Introduction

Basic physical mechanisms that are complicated can often be studied with the aid of simple quantum mechanical models that exhibit the effects of interest. We have been interested in energy exchange between two-level systems and an oscillator under conditions where the two-level system energy is much greater than the oscillator energy. This problem first became of interest in quantum mechanics in the course of early NMR studies by Bloch and Siegert [1]. A strong applied magnetic field causes a splitting of spin levels, creating a two-level system in the case of a spin ½ nucleus. A dynamical transverse field causes transitions between the upper and lower levels of the two-level system. Early work on this problem was done using the Rabi Hamiltonian, in which the oscillator appears in the problem as a time-dependent interaction potential [1,2]. In the mid 1970s, Cohen-Tannoudji and colleagues introduced the spin-boson model, in which a quantum model is used for the oscillator [3].

The spin-boson model in recent years has been used to model electromagnetic interactions between atomic or molecular systems and radiation fields, as well as serving as a workhorse model for testing new kinds of approximations or formulations. By now, there are hundreds of papers on spin-boson and related models, and the interest in such models as basic physical models is only increasing.

We have been interested in the spin-boson model and the closely related Dicke model (which generalizes the spin-boson model to include many identical two-level systems) in the multiphoton regime, in order to focus on the coherent exchange of many small oscillator quanta for a single large two-level system quantum. In the course of this work, we have exploited a rotation which splits the Hamiltonian into different pieces which have simple functionality, which allows us to understand multiphoton interactions simply. We have explored models in which a great many oscillator quanta are exchanged coherently, and we have found variants of the basic models in which energy exchange is greatly accelerated. Some of these results will be reviewed in what follows.

Spin-boson and Dicke models

The spin-boson model is described by the Hamiltonian

$$\hat{H} = \Delta E \frac{\hat{S}_z}{\hbar} + \hbar\omega_0 \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) + V\left(\hat{a}^\dagger + \hat{a} \right) \frac{2\hat{s}_x}{\hbar}$$

The first term describes the energy levels of a two-level system, and the second describes a simple harmonic oscillator. The two quantum systems are coupled linearly, as accounted for by the remaining term. The transition energy of the two-level system is ΔE, and the oscillator energy is $\hbar\omega_0$. In the multiphoton regime the oscillator energy is much less than the two-level system energy

$$\hbar\omega_0 \ll \Delta E$$

The Dicke model is very closely related. We may write

$$\hat{H} = \Delta E \frac{\hat{S}_z}{\hbar} + \hbar\omega_0 \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) + V\left(\hat{a}^\dagger + \hat{a} \right) \frac{2\hat{S}_x}{\hbar}$$

In the Dicke model, we have many spin operators

$$\hat{S}_\alpha = \sum_j \hat{s}_\alpha^{(j)}$$

where

$$\hat{s}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad\qquad \hat{s}_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Viewed in this way, the spin-boson model represents the s=1/2 limit of the Dicke model.

Unitary transformation

We can rotate the Hamiltonian using a unitary transformation

$$\hat{H}' = \hat{U}^\dagger \hat{H} \hat{U}$$

where

$$\hat{U} = \exp\left\{ -\frac{i}{2} \tan^{-1}\left(\frac{2U\left(\hat{a}^\dagger + \hat{a} \right)}{\Delta E} \right) \frac{2\hat{s}_y}{\hbar} \right\}$$

to produced a rotated Hamiltonian of the form

$$\hat{H}' = \hat{H}_0 + \hat{V} + \hat{W}$$

This rotated Hamiltonian is composed of an "unperturbed" part H_0

$$\hat{H}_0 = \sqrt{\Delta E^2 + 4V^2 \left(\hat{a}^\dagger + \hat{a} \right)^2} \, \frac{\hat{s}_z}{\hbar} + \hbar\omega_0 \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right)$$

This unperturbed Hamiltonian is interesting for a variety of reasons: it gives a reasonable description of the states and energy eigenvalues of the system; and it explicitly does not include effects associated with multiphoton energy exchange effects. In addition, there is a perturbation V

$$\hat{V} = \frac{i}{2}\hbar\omega_0\frac{U}{\Delta E}\left\{\frac{1}{1+\left(\dfrac{2V\left(\hat{a}^\dagger+\hat{a}\right)}{\Delta E}\right)^2}\left(\hat{a}^\dagger-\hat{a}\right)+\left(\hat{a}^\dagger-\hat{a}\right)\frac{1}{1+\left(\dfrac{2V\left(\hat{a}^\dagger+\hat{a}\right)}{\Delta E}\right)^2}\right\}\frac{2\hat{s}_y}{\hbar}$$

This operator is interesting because it mediates the multiphoton transitions that we are interested in studying. The final term *W* that appears in the rotated Hamiltonian is small for problems of interest to us, so we ignore it.

Basis states in the rotated problem

Using this rotation, we are able to understand the energy levels and associated dynamical effects simply. The basis states of the unperturbed rotated Hamiltonian satisfy

$$E\Phi = \hat{H}_0\Phi$$

These basis states contain a spin part and an oscillator part

$$\Phi = \left|s,m\right\rangle u\left(y\right)$$

Where the spin function is for s=1/2, and describes lower (m=-1/2) and upper (m=1/2) states of the two-level system. The oscillator function u(y) satisfies

$$Eu\left(y\right) = \frac{\hbar\omega_0}{2}\left(-\frac{d^2}{dy^2}+y^2\right)u\left(y\right)+m\sqrt{\Delta E^2+8V^2y^2}\,u\left(y\right)$$

When the oscillator is very highy excited, so that the loss or gain of a two-level system quanta does lead to a significant perturbation of the oscillator, then the energy levels are approximately

$$E_{m,n} = \Delta E\left(g\right)m+\hbar\omega_0\left(n+\frac{1}{2}\right)$$

Here, *g* is the dimensionless coupling constant

$$g = \frac{V\sqrt{n}}{\Delta E}$$

The associated interpretation is that the oscillator causes the two-level system transition energy to increase, but the two-level system does not impact the oscillator. This picture corresponds to the approximation

$$u\left(y\right) = \phi_n\left(y\right) \qquad \Delta E\left(g\right) = \left\langle\phi_n\left|\sqrt{\Delta E^2+8U^2y^2}\right|\phi_n\right\rangle$$

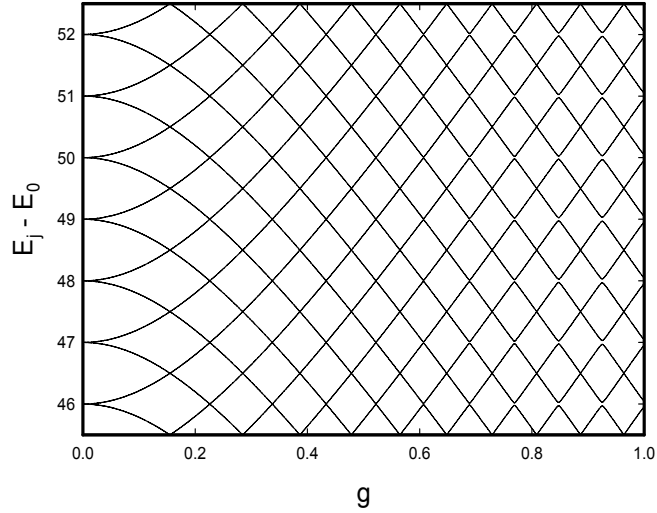which provides an excellent starting place for understanding energy exchange.

Figure 1 – Energy levels of the spin-boson problem as a function of the dimensionless coupling strength for $\Delta E = 11 \ \hbar\omega_0$. The energy is given in units of $\hbar\omega_0$, with an offset.

Coherent multiphoton energy exchange

The energy eigenvalues of the spin-boson Hamiltonian are shown above. In the absence of coupling (g=0), two energy eigenvalues appear spaced every $\hbar\omega_0$. As g increases, the upper level of the two-level system goes up, the lower level goes down, and one sees that the different energy level run into one another. In some cases they cross, and in other cases they anticross. The resonance condition is given approximately by

$$\Delta E\left(g\right) \ = \ \Delta n \ \hbar\omega_0$$

Anticrossings occur when Δn is odd (a selection rule for this model), which corresponds to a mixing between states. Near an anticrossing, we can describe the system using a simple superposition of two states

$$\Psi \ = \ c_0\Phi_{1/2,n} + c_1\Phi_{-1/2,n+\Delta n}$$

The splitting between the two states can be found using perturbation theory in the rotated picture to be

$$\delta E_{min} \ = \ 2\left|\left\langle\Phi_{1/2,n}\left|\hat{V}\right|\Phi_{-1/2,n+\Delta n}\right\rangle\right|$$

Although this constitutes a simple approximation in the rotated version of the problem, it captures the level splitting (and hence also the dynamics) at the anticrossings, as illustrated in Figure 2.
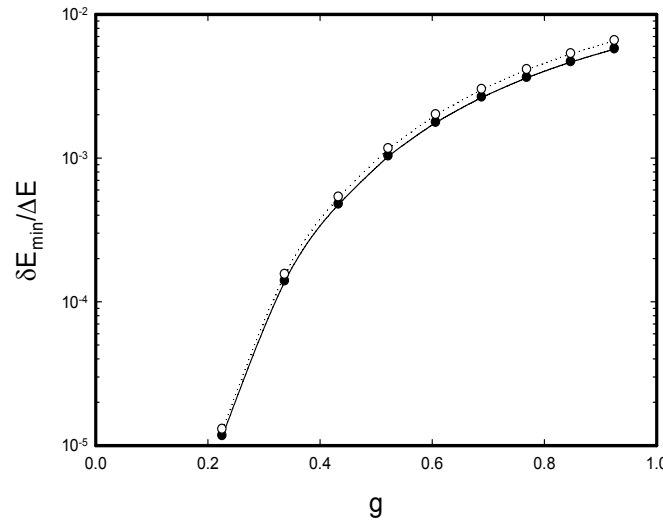
Figure 2 – Level splittings from a full computation using the spin-boson model at large n for $\Delta E = 11\ \hbar\omega_0$ (solid circles), compared with two-state degenerate perturbation theory in the rotated problem (open circles).

On resonance, the probability oscillates between the two basis states; we may write

$$|c_0|^2 \;=\; \cos^2\frac{\delta E_{\min}t}{2\hbar} \qquad\qquad |c_1|^2 \;=\; \sin^2\frac{\delta E_{\min}t}{2\hbar}$$

The level splitting at the anticrossings determines the rate at which coherent multiphoton energy exchange occurs in the spin-boson model.

Coherent multiphoton energy exchange in the Dicke model

The discussion so far provides us with a simple way to think about coherent multiphoton energy exchange in the spin-boson model. Using the rotation, we obtain a satisfactory set of basis states that describe a dressed two-level system with a transition energy increased due to the interaction with the oscillator. We then make use of the perturbation operator, which allows us to treat multiphoton transitions on the same footing as single photon transitions. Simple degenerate perturbation theory then gives us the relevant dynamics.

The problem becomes more complicated when there are many two-level systems. Diagonalization of the Dicke Hamiltonian results in a much larger number of states with a more complicated structure of the energy levels. However, the Dicke model itself describes a set of identical two-level systems interacting with an oscillator, so one would expect that all of the two-level systems should exchange energy under pretty much the same conditions that a single one should. The only significant difference appears to be that the oscillator can gain or lose much more energy, which can lead to a change in the dressed two-level system energy, which in turn can destroy the resonance condition.

We can make progress by first computing energy levels for the full Dicke model in order to see what happens near resonance. Results are shown in Figure 3. One sees that many energy levels approach an anticrossing; they are roughly equispaced on resonance (the level splitting is about the same as in the spin-boson model).
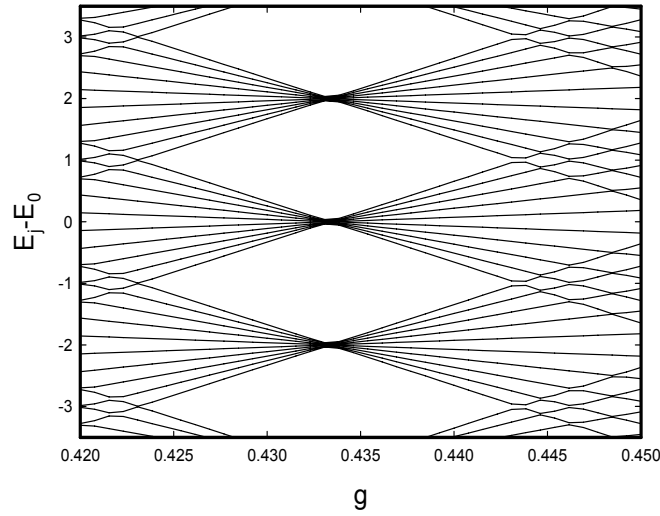
Figure 3 – Level anticrossings for the Dicke model as a function of the dimensionless coupling constant. In this case there are 10 energy levels (corresponding to 9 two-level systems) that approach an anticrossing. Relative energies are in units of $\hbar\omega_0$. Only levels corresponding with states of the same parity are shown to simplify the figure. The anticrossing in this case corresponds to a 17 quantum resonance for a model with $\Delta E = 11\ \hbar\omega_0$.

We can develop a dynamical solution for the Dicke model from a finite basis expansion using the states that anticross at a single anticrossing. Such a solution can be written in the form

$$\Psi = \sum_j c_j e^{-iE_j t/\hbar} \Phi_j$$

We can select values for the coefficients c_j to start all of the two-level systems in highly excited states, and then watch the evolution of the coupled system. In the example considered below, the basis states are very complicated, so it is useful to find a simple way to present the resulting dynamics. It is convenient to focus on the probabilities associated with the Dicke number M (for maximum M, all of the two-level systems are excited, and for minimum M, all of them are in the ground state), and the oscillator number n. We may write

$$p_M(t) = \sum_j \sum_k \sum_n c_j^* c_k e^{i(E_j - E_k)t/\hbar} \Phi_j^*(M,n) \Phi_k(M,n)$$

$$p_n(t) = \sum_j \sum_k \sum_M c_j^* c_k e^{i(E_j - E_k)t/\hbar} \Phi_j^*(M,n) \Phi_k(M,n)$$

Results for these probabilities as a function of time are shown in Figures 4 and 5. One sees in this computation that 100 two-level systems exchange about 1700 oscillator quanta back and forth slowly.
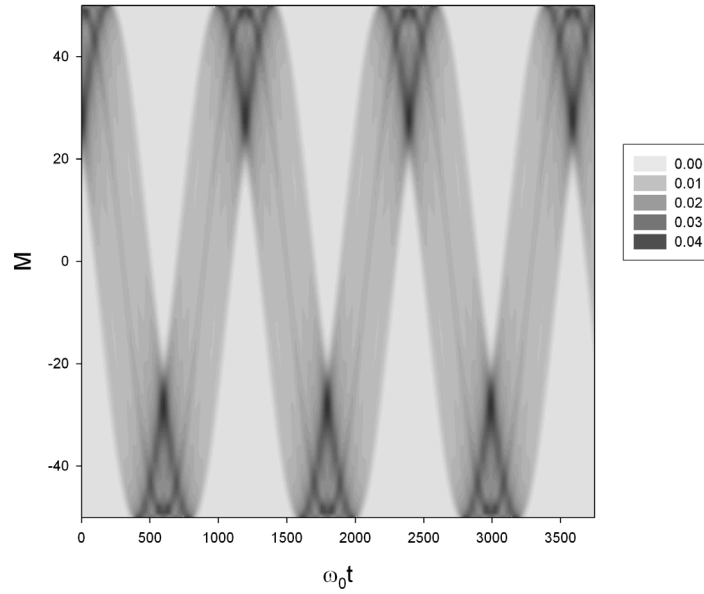
Figure 4 – Probability $p_M(t)$ as a function of $\omega_0 t$ for 100 two-level systems in a Dicke model exchanging energy with a low energy oscillator.
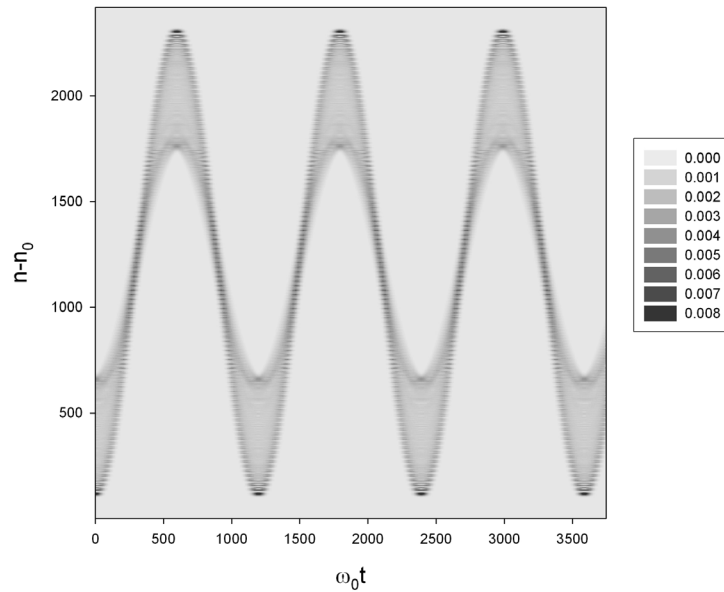

Figure 5 – Probability $p_n(t)$ as a function of $\omega_0 t$ for 100 two-level systems in a Dicke model exchanging energy with a low energy oscillator.

Simple models for coherent multiphoton energy exchange

In the computations presented above, we used a brute force numerical diagonalization of the Dicke Hamiltonian that involved about 120,000 individual $|M,n\rangle$ basis states. Had we wished to perform similar computations for more two-level systems, or for a larger ratio of two-level energy

to oscillator energy, the number of states would have been even larger. Since the computational resources for such computations quickly becomes prohibitive, it would be useful to develop simpler models that capture what is important in coherent multiphoton energy exchange.

One approach is to focus on the nearly degenerate basis states that we used above. This suggests a dynamical basis in the rotated version of the problem of the form

$$\Psi' = \sum_M c_M(t)\Phi'_{M,n-M\Delta n}$$

where we keep only terms that approximately satisfy the resonance condition

$$\Delta E(g)M + \hbar\omega_0 \, \Delta n \, M = \text{constant}$$

The expansion coefficients then approximately satsify

$$i\hbar\frac{d}{dt}c_M = \left(h_0 + h_1 M + h_2 M^2\right)c_M + v\sqrt{(S+M)(S-M+1)}c_{M-1} + v\sqrt{(S-M)(S+M+1)}c_{M+1}$$

The energy eigenvalues of the rotated H_0 Hamiltonian are in general complicated, but for coherent multiphoton energy exchange to occur, they must be nearly degenerate. We have found that keeping terms up to second order captures much of the effects of detuning when the oscillator is off of resonance, and effects due to a shift in resonance associated with the gain or loss of oscillator quanta. The matrix elements of the perturbation operator V are also complicated, but the most important dependence as a function of M comes from the Dicke factors which arise in lowest-order multiphoton coupling with this operator. We have been able to obtain good agreement with the oscillation frequency, amount of energy exchange, and in the coherence of the coherent multiphoton energy exchange process using this model as compared with results from the full Dicke model.

We have also found a closely related classical model which can also be used. This model can be written as

$$\frac{d}{dt}\mathbf{S}(t) = \frac{d\theta}{dt}\mathbf{n}\times\mathbf{S}(t)$$

where

$$\langle\mathbf{S}(t)\rangle \rightarrow \mathbf{S}(t) \qquad n_x h\frac{d\theta}{dt} = 2v_0 \qquad n_z h\frac{d\theta}{dt} = h_1 + 2h_2 S_z$$

This model gives an approximate description for the evolution of expectation values for the reduced quantum model above.

Enhancement of coherent multiphoton energy exchange

The rotation discussed above for the spin-boson problem generalizes directly to the Dicke problem by a simple replacement of single spin operators with many spin operators, leading to a perturbation operator V that is proportional to S_y. Because of this, only a single Dicke factor appears in the associated matrix elements, which is why we used only a single Dicke factor in the coupling term of the simplified model outlined above. This seems perhaps to be odd, since we are talking about interactions in which many interactions occur, and we would expect each

individual interaction to produce a Dicke factor, resulting in the product of many Dicke factors overall.

To investigate this, we decided to focus on coherent multiphoton energy exchange in the weak coupling limit where we might make use of perturbation theory to understand how this works. In the case of a five photon transition, there are in general twelve states that are involved in connecting one state to its nearest indirectly-coupled degenerate neighbor. This situation is shown in Figure 6.
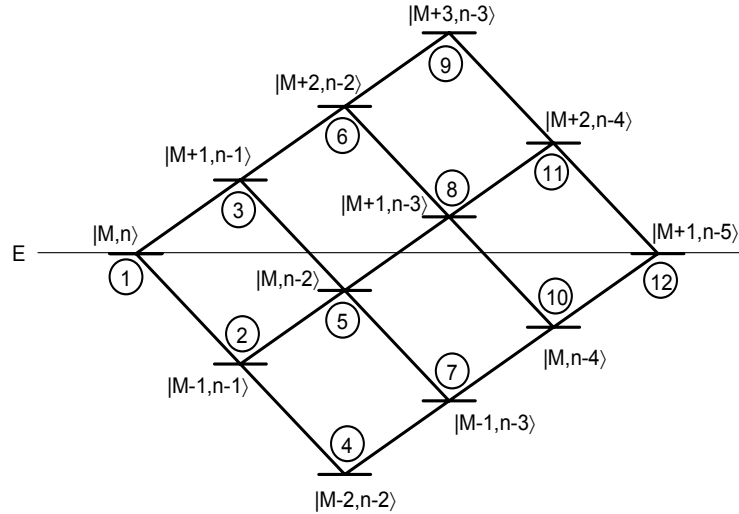

Figure 6 – Schematic of basis states involved in the lowest-order indirect coupling in the case of a 5 photon transition.

There are 10 different pathways that contribute at lowest order to the indirect coupling matrix element. We may write

$$V_{1,12} = \frac{V_{1,2}V_{2,4}V_{4,7}V_{7,10}V_{10,12}}{(E-H_2)(E-H_4)(E-H_7)(E-H_{10})} + \cdots$$

where we have indicated one of the terms corresponding to one of the paths. Each V_{ij} that appears in the numerator contains a Dicke factor. When we sum up the different contributions from all of the different paths, we obtain

$$V_{1,12} = \frac{625}{64}\frac{V^5}{\Delta E^4}\sqrt{n(n-1)(n-2)(n-3)(n-4)}\sqrt{(S-M)(S+M+1)}$$

Only a single Dicke factor appears in the resulting summation. This comes about because there is destructive interference which occurs between the different pathways.

If this destructive interference could be removed, then the resulting indirect coupling would be greatly increased. In this case, coherent multiphoton energy exchange would be greatly

enhanced. If we augment the model with loss, then the destructive interference can be eliminated. In the simplest loss model, we might assume that all intermediate states with a basis energy less than E is unstable, and decays very rapidly. In the limit of infinitely fast decay, the resulting indirect coupling is

$$V_{1,12} = \frac{625}{64}\frac{V^5}{\Delta E^4}\sqrt{n(n-1)(n-2)(n-3)(n-4)}\sqrt{(S-M)(S+M+1)}\,F(S,M)$$

where

$$F(S,M) = \frac{1}{18}\left[\begin{array}{c}5S^4+10S^3-S^2\left(10M^2-8M-22\right)-S\left(10M^2-8M-17\right)+\\ \left(5M^4-8M^3-14M^2+17M+18\right)\end{array}\right]$$

This is illustrated in Figure 7 in the case of 100 two-level systems (S=50). One sees more than 6 orders of magnitude increase in the indirect coupling in this case, which corresponds to a commensurate increase in the coherent multiphoton energy exchange rate.
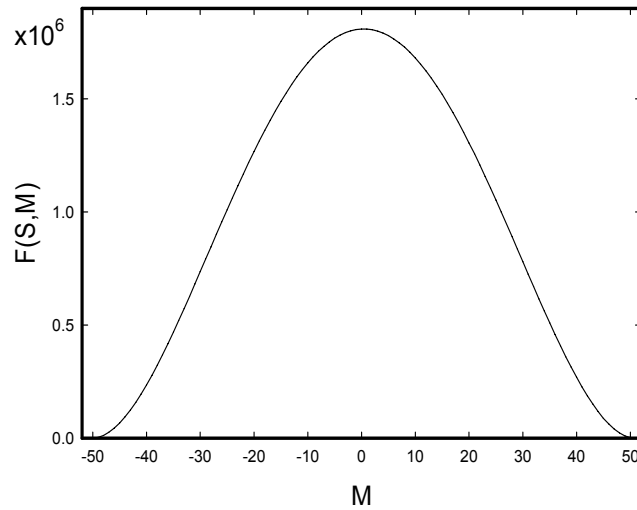

Figure 7 – Enhancement for coherent multiphoton energy exchange in a lossy model where the destructive interference is removed. Results are for 5 photon exchange and 100 two-level systems.

References

1. F. Bloch and A. Siegert, "Magnetic resonance for nonrotating fields," *Phys. Rev.* **57**, 522 (1940).

2. J. H. Shirley, "Solution to the Schrodinger equation with a Hamiltonian periodic in time," *Phys. Rev.* **138**, B979 (1965).

3. C. Cohen-Tannoudji, J. Dupont-Roc, and C. Fabre, "A quantum calculation of the higher order terms in the Bloch-Siegert shift," *J. Phys. B* **6**, L214 (1973).

4. P. L. Hagelstein and I. U. Chaudhary, "Level splitting in association with the multiphoton Bloch-Siegert shift," *J. Phys. B* **41** 035601 (2008).

5. P. L. Hagelstein and I. U. Chaudhary, "Multiphoton Bloch-Siegert shifts and level splittings in spin one systems," *J. Phys. B* **41** 035602 (2008).

6. P. L. Hagelstein and I. U. Chaudhary, "Multiphoton Bloch-Siegert shifts and level splittings in a three-level system," *J. Phys. B* **41** 105603 (2008).

7. P. L. Hagelstein and I. U. Chaudhary, "Excitation transfer in two two-level systems coupled to an oscillator," *J. Phys. B* **41** 135501 (2008).

8. P. L. Hagelstein and I. U. Chaudhary, "Coherent multiphoton energy exchange between a Dicke system and an oscillator," submitted to *J. Phys. B*.

9. P. L. Hagelstein and I. U. Chaudhary, "Electron mass shift in nonthermal systems," *J. Phys. B* **41** 125001 (2008).