Research Article

Local Approximation for the Lossy Spin–boson Model

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Abstract

We are interested in the problem of coherent energy exchange in the spin-boson model augmented with loss, in the limit of infinite loss. This model is interesting because it predicts rapid coherent energy exchange under conditions when the transition energy of the two-level systems is much greater than the characteristic energy of the oscillator. Here we introduce the local approximation, in which we assume that the matrix elements change little when an energy exchange event occurs. This approximation results in a periodic system when a resonance condition is satisfied, which is much easier to solve than the original problem. We consider a model problem where we analyze the self-energy and indirect coupling matrix elements numerically and in the local approximation, with good agreement. Systematic results from the local approximation are obtained for the self-energy and indirect coupling matrix elements in models where 3, 5, 7, 9, and 11 quanta are exchanged.
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1. Introduction

There have been a great many experiments which indicate that excess energy is produced in the Fleischmann–Pons experiment [1,2] and its variants. The amount of energy observed in some of these experiments is prodigious, with no obvious commensurate chemical processes observed. Since there has been measured ^{4}He in amounts proportional to the energy produced [3–5], with an associated Q-value near 24 MeV [6], one possible conclusion is that there is some kind of new nuclear reaction process occurring. The conundrum that arises in such a proposal is that known exothermic nuclear reactions put the reaction energy into energetic nuclear particles. In the Fleischmann–Pons experiment, there simply aren't energetic nuclear particles in amounts commensurate with the energy produced [7]. Consequently, conventional

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nuclear reactions that appear in the nuclear physics literature in general cannot be candidates to account for the excess heat effect.

If so, then the question arises as to what reactions or new physical processes can be consistent with these experimental observations? It seems the outstanding theoretical problem which must be faced involves the conversion of a very large MeV-level nuclear quantum of energy into a very large number of eV-level or meV-level quanta.

If we adopt such a point of view, then the recent results from two-laser experiments [8,9] perhaps begin to make sense. Excess power is observed when the cathode is stimulated by two weak laser beams, and the response depends on the frequency difference between the two laser frequencies. Two of the frequencies at which strong responses are observed correspond to the Γ-point (8 THz) and L-point (15 THz) of the optical phonon mode dispersion curve of PdD. The excess power in these experiments is seen in many cases to persist when the lasers are turned off. Some power is put into one of the these modes by the lasers, which initially stimulates excess power production. If excess power continues when the lasers are turned off, we might infer that some of the energy which is being produced in the reaction is going into the mode that has been stimulated. This could be verified by Raman measurements, but such experiments have not yet been attempted.

From experiment, a picture seems to emerge in which a new kind of nuclear reaction process occurs, in which the reaction energy is communicated to the optical phonon modes. Such an effect is unprecedented, which makes the theoretical problem of model development that much harder. Nevertheless, we have managed to construct new models based on two-level systems coupled to an oscillator, which exhibit a much accelerated coherent energy exchange effect involving the fractionation of a large energy quantum into a great many low energy quanta.

The simplest version of the model is the spin-boson model augmented with loss, which we have introduced in earlier publications. We have demonstrated the new coherent energy exchange effect using perturbation theory [10], and we have also presented a second-order formulation of the model [11] which allows us to think about the model in terms of a set of ordered nearly degenerate states with nearest neighbor coupling. In these papers, we have begun the analysis of the model, introducing tools that help us understand and analyze important properties. Our goal ultimately is to understand how coherent energy exchange works in a regime relevant to the Fleischmann–Pons experiment, and in this work we take a big step in that direction. In this paper, we introduce the local approximation, which provides us with a powerful tool to analyze coherent energy exchange when the coupling is strong, and also when a larger number of oscillator quanta are exchanged.

2. Local Approximation for the Lossy Spin-boson Model

As we have discussed in earlier works, the lossy spin-boson model is described by the Hamiltonian [10]

$$\hat{H} = \Delta E \frac{\hat{S}_z}{\hbar} + \hbar\omega_0 \hat{a}^\dagger \hat{a} + V(\hat{a}^\dagger + \hat{a})\frac{2\hat{S}_x}{\hbar} - i\frac{\hbar}{2}\hat{\Gamma}(E),\tag{1}$$

where ΔE is the transition energy of the two-level systems, where $\hbar\omega_0$ is the oscillator energy, and where V is the coupling strength. Loss is included through the second-order $-i\hbar\hat{\Gamma}(E)/2$ term that comes from a Brillouin–Wigner formulation (see [10]). Eigenfunctions of the coupled two-level systems and oscillator can be found from the solution of the eigenvalue problem

$$E\Psi = \hat{H}\Psi.\tag{2}$$

2.1. Finite basis approximation

We can make use of a finite basis approximation for the associated wave function in terms of product basis states according to

$$\Psi = \sum_m \sum_n c_{m,n}|S,m\rangle|n\rangle. \tag{3}$$

We can use this to develop the above eigenvalue equation in terms of the expansion coefficients according to

$$
\begin{aligned}
Ec_{m,n} = & \left(\Delta E m + \hbar\omega_0 n - i\frac{\hbar}{2}\Gamma(E)\right)c_{m,n} + V\sqrt{n+1}\sqrt{(S-m)(S+m+1)}c_{m+1,n+1} \\
& + V\sqrt{n}\sqrt{(S-m)(S+m+1)}c_{m+1,n-1} + V\sqrt{n+1}\sqrt{(S+m)(S-m+1)}c_{m-1,n+1} \\
& + V\sqrt{n}\sqrt{(S+m)(S-m+1)}c_{m-1,n-1}.
\end{aligned} \tag{4}
$$

2.2. Limit of many oscillator quanta and two-level systems

In the event that n is very large, then

$$\sqrt{n+1} \approx \sqrt{n}. \tag{5}$$

If S is very large, and if m is not close to $\pm S$, then

$$\sqrt{(S-m)(S+m+1)} \approx \sqrt{S^2 - m^2}, \qquad \sqrt{(S+m)(S-m+1)} \approx \sqrt{S^2 - m^2} \tag{6}$$

Under these approximations, the coupling coefficients to the nearby states are the same, so that the eigenvalue equation for the expansion coefficients is approximately

$$
\begin{aligned}
Ec_{m,n} = & \left[\Delta E m + \hbar\omega_0 n - i\frac{\hbar}{2}\Gamma(E)\right]c_{m,n} \\
& + V\sqrt{n}\sqrt{S^2 - m^2}\left(c_{m+1,n+1} + c_{m+1,n-1} + c_{m-1,n+1} + c_{m-1,n-1}\right).
\end{aligned} \tag{7}
$$

2.3. Local approximation in terms of g

We recall that the dimensionless coupling constant g is given by

$$g = \frac{V\sqrt{n}\sqrt{S^2 - m^2}}{\Delta E}. \tag{8}$$

The approximate eigenvalue equation can be written in terms of the dimensionless coupling constant as

$$
\begin{aligned}
\frac{E}{\Delta E}c_{m,n} = & \left(1 + \frac{\hbar\omega_0}{\Delta E} - i\frac{\hbar\Gamma(E)}{2\Delta E}\right)c_{m,n} \\
& + g\left(c_{m+1,n+1} + c_{m+1,n-1} + c_{m-1,n+1} + c_{m-1,n-1}\right).
\end{aligned} \tag{9}
$$

Although g is dependent on m, we can simplify the problem significantly if we consider it to be a constant. The eigenvalue equation that results constitutes a local approximation, allowing us to obtain approximate basis state energies and indirect coupling coefficients.

2.4. Hamiltonian associated with the local approximation

We can write down a Hamiltonian for this local approximation as

$$\hat{H} \; = \; \Delta E \frac{\hat{S}_z}{\hbar} + \hbar\omega_0 \hat{a}^\dagger \hat{a} + g\Delta E \left(\hat{\delta}_+^n + \hat{\delta}_-^n \right)\left(\hat{\delta}_+^m + \hat{\delta}_-^m \right) - i\frac{\hbar}{2}\hat{\Gamma}(E), \tag{10}$$

where the $\hat{\delta}$ operators satisfy

$$\hat{\delta}_\pm^n |n\rangle \; = \; |n \pm 1\rangle, \tag{11}$$

$$\hat{\delta}_\pm^m |S, m\rangle \; = \; |S, m \pm 1\rangle. \tag{12}$$

3. Periodicity

An important feature of the Hamiltonian in the local approximation is that it is invariant under translations of the form

$$\hat{T}_\pm |S, m\rangle|n\rangle \; = \; |S, m \pm 1\rangle|n \mp \Delta n\rangle, \tag{13}$$

when the resonance condition holds

$$\Delta E \; = \; \Delta n\, \hbar\omega_0 \tag{14}$$

for odd Δn.

3.1. Bloch's theorem

The Hamiltonian is invariant under the energy-preserving translations of the $\hat{T}_\pm$ operators, so we know that Bloch's theorem applies. The eigenfunctions $\Phi_{m,n}$ of the local Hamiltonian satisfy the time-independent Schrödinger equation

$$\hat{H}\Phi_{m,n} \; = \; E\Phi_{m,n}. \tag{15}$$

In the local approximation with odd integer Δn, the Hamiltonian commutes with the translation operators

$$[\hat{T}_\pm, \hat{H}] \; = \; 0. \tag{16}$$

Hence it is possible to find solutions which are eigenfunctions of both operators

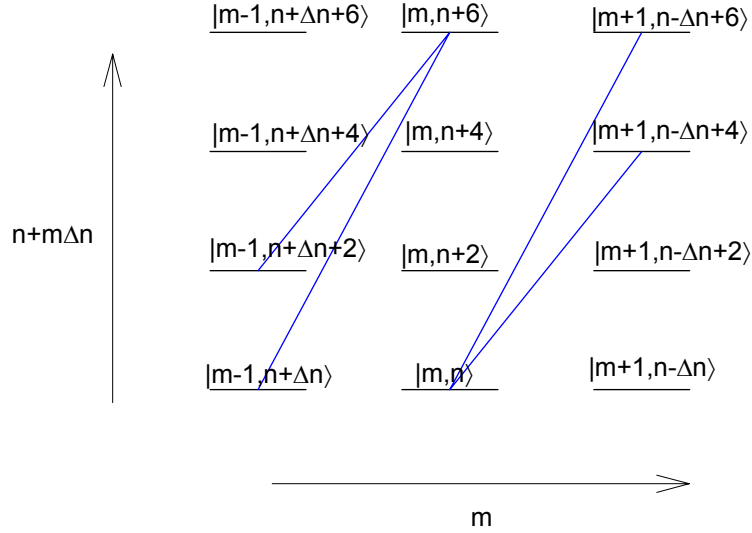$$\hat{H}\Phi_{m,n} \; = \; E\Phi_{m,n}, \tag{17}$$

Figure 1.   Levels and selected couplings in m and $n + m\Delta n$ basis with $\Delta n = 5$, plotted using m and $n + m\Delta n$ (proportional to the energy) axes. State $|m, n + 6\rangle$ is coupled to higher energy states $|m + 1, n + 6 \pm 1\rangle$, although this coupling is not shown.

$$\hat{T}_+ \Phi_{m,n} = C \Phi_{m,n}. \tag{18}$$

These solutions can be written in the form

$$\Phi_{m,n} = e^{im\phi} u_{m,n}, \tag{19}$$

where the $u_{m,n}$ are periodic in m. As a result, the energy eigenvalues can be described as a set of bands in ϕ from the eigenvalue equation

$$E(\phi) e^{im\phi} u_{m,n} = \hat{H} e^{im\phi} u_{m,n}. \tag{20}$$

3.2. Reduced problem and boundary conditions

Since the problem is periodic under the local Hamiltonian, we can reduce the problem by working with a single column of states such as plotted in Fig. 1. We need only include the states $|m, n\rangle$, $|m, n + 2\rangle$, $\cdots$ explicitly. The phase factors that result in the Bloch solution relate the phase of a basis state with one value of m to the phase of the basis state at the same energy at a neighboring value of m. So, a Bloch state solution can be developed from a set of expansion coefficients associated with the basis states in a single column, knowing that the expansion coefficients for the basis states in neighboring columns differ only by a single phase factor for each column.

4. Product solution

The discussion above suggests that a convenient product solution can be constructed using

$$\Psi \ = \ \sum_m \sum_n d_m v_{n+m\Delta n} |S, m\rangle |n + m\Delta n\rangle \tag{21}$$

assuming large S with m away from $\pm S$, and large n. Since the index of the v coefficients is proportional to the basis state energy, it is unaffected by $\hat{T}_\pm$ translations. Hence we can implement the phase factors associated with the Bloch states in the d_m coefficients by taking

$$d_m \ = \ e^{im\phi}. \tag{22}$$

The local Hamiltonian couples states with m and n indices that differ by one unit; however, when we line the states up according to their energy (which is useful in the local approximation), then this coupling appears to connect relatively distant states as indicated in Fig. 1.

4.1. Self-energy

Starting with the basis expansion above, we can isolate the v coefficients by taking advantage of orthogonality

$$\langle m', n' | m, n \rangle \ = \ \delta_{m',m} \delta_{n',n}. \tag{23}$$

The eigenvalue equation associated with the expansion coefficients can be written as

$$E(\phi) d_m v_{n+m\Delta n} \ = \ \left[\Delta E m + n\hbar\omega_0 - i\frac{\hbar}{2}\hat{\Gamma}(E) \right] d_m v_{n+m\Delta n}$$
$$+ g\Delta E \Big[d_{m+1}(v_{n+1+(m+1)\Delta n} + v_{n-1+(m+1)\Delta n})$$
$$+ d_{m-1}(v_{n+1+(m-1)\Delta n} + v_{n-1+(m-1)\Delta n}) \Big]. \tag{24}$$

If we focus on the coefficients corresponding to the column with $m = 0$ and use $d_m = \exp(im\phi)$, we obtain

$$E(\phi) v_n \ = \ \left[n\hbar\omega_0 - i\frac{\hbar}{2}\hat{\Gamma}(E) \right] v_n$$
$$+ g\Delta E \Big[e^{i\phi}(v_{n+\Delta n+1} + v_{n+\Delta n-1}) + e^{-i\phi}(v_{n-\Delta n+1} + v_{n-\Delta n-1}) \Big]. \tag{25}$$

The lowest energy solution of this eigenvalue equation gives the self-energy in the local approximation.

4.2. Indirect coupling matrix element

Under conditions that are of interest to us in the development of models relevant to the excess heat effect in the Fleischmann–Pons experiment, the indirect coupling between nearly degenerate states is weak. In the local approximation, a second-order formulation that isolates the nearly degenerate states would result in degenerate states when Δn is an odd integer. The associated eigenvalue equation is of the form
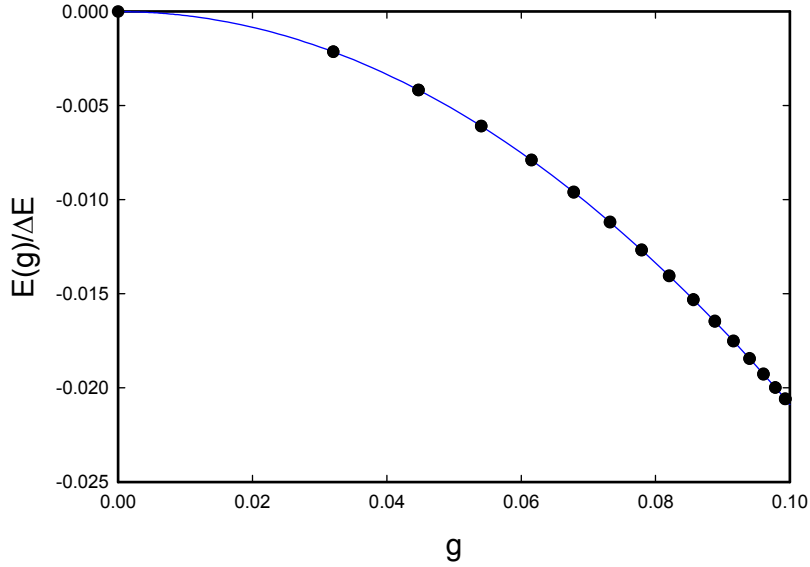
Figure 2. Self-energies for the nearly degenerate basis states of the test problem (black circles) and for the local approximation (blue line).

$$Ed_m = E_0 d_m + V_{\text{eff}}(d_{m-1} + d_{m+1}). \tag{26}$$

It is possible to obtain a useful version of such an equation from the model under consideration above (but this will be of more interest in a later paper, so we defer the associated discussion).

We can solve this equation using

$$d_m = e^{im\phi} \tag{27}$$

consistent with the phase factor that we used above from Bloch's theorem. The associated energy eigenvalue is

$$E(\phi) = E_0 + 2V_{\text{eff}} \cos\phi. \tag{28}$$

As a result, if we were to solve the eigenvalue equation in the local approximation for two values of ϕ, then we could determine the indirect coupling coefficient in the weak coupling approximation. For example, if we take ϕ values of 0 and π, then we obtain

$$E(0) - E(\pi) = 4V_{\text{eff}}. \tag{29}$$

We have used this to obtain numerical estimates for the indirect coupling matrix element for the restricted basis version of the infinite loss model with success.
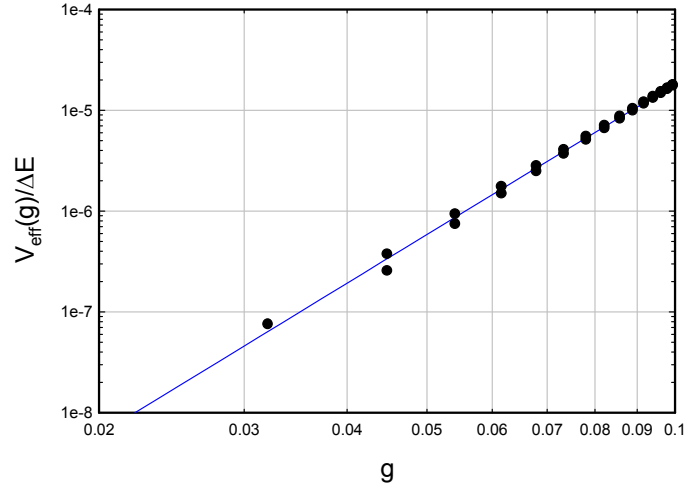
Figure 3. Indirect coupling matrix elements for the nearly degenerate basis states of the test problem (black circles) and for the local approximation (blue line).

5. Model Problem

The local approximation described above allows us to develop approximate results for the self-energy and indirect coupling matrix elements for the lossy spin-boson model. Since it is an approximation, we are interested in whether it can give good results. To explore this, we developed a model problem in which we can compare the approximate results with exact numerical results.

5.1. Problem specification

For the test problem, we chose

$$\frac{\Delta E}{\hbar \omega_0} = 5 \tag{30}$$

with

$$S = 19.5, \tag{31}$$

which corresponds to 39 two-level systems. We took the coupling strength V to satisfy

$$\frac{V\sqrt{n}S}{\Delta E} = 0.1 \tag{32}$$

for which the maximum dimensionless coupling strength g is close to 0.10. We have taken the lossy spin-boson model in the limit of infinite loss, using a restricted basis approximation [11].
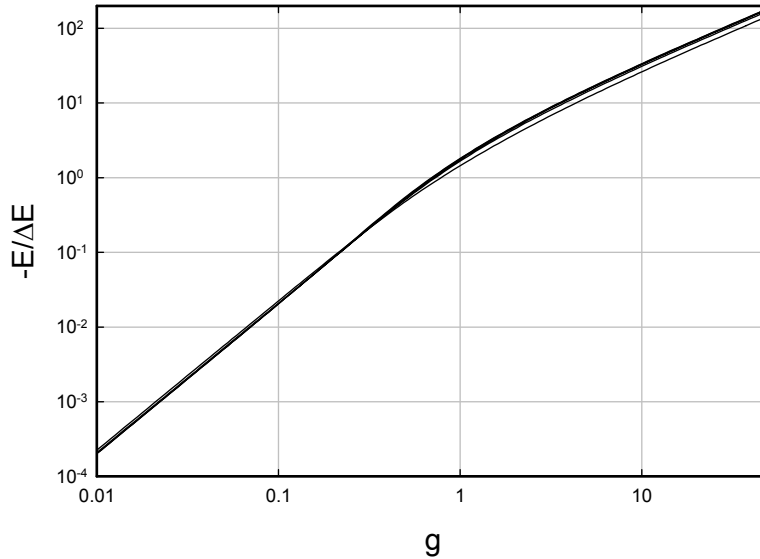
Figure 4.　Self-energy as a function of g for $\Delta n = 3,5,7,9,11$ ($n = 3$ is the bottom curve, and $n = 11$ is the top).

5.2. Second-order formulation

In a previous paper we described a second-order formulation for the lossy spin-boson problem [11]. The advantage of this formulation is that we are able to reduce the original complicated Hamiltonian into a conceptually simpler one that focuses on a set of nearly degenerate states that are coupled indirectly. This formulation can be represented through the second-order Hamiltonian

$$\mathbf{H}(E) \;=\; \mathbf{H}_a + \mathbf{V}_{ab} \cdot (E - \mathbf{H}_b)^{-1} \cdot \mathbf{V}_{ba}, \tag{33}$$

which we can evaluate numerically to determine the self-energies and indirect matrix elements.

For this calculation, we took 50 energy points for the energy in the denominator and evaluated the self-energies and indirect coupling matrix elements between nearest neighbors. Then we interpolated for self-consistency for each state to get the self-energies. Based on this interpolation we obtained accurate values for the indirect coupling matrix elements.

5.3. Comparison of the self-energy

To compare the results from the two models, we needed to develop an estimate for the local coupling strength. Our procedure was to sum the coupling matrix elements out of one of the initial degenerate basis states of the original full Hamiltonian, and then divide by the product of ΔE and the number of couplings. This produces an approximate local g defined by
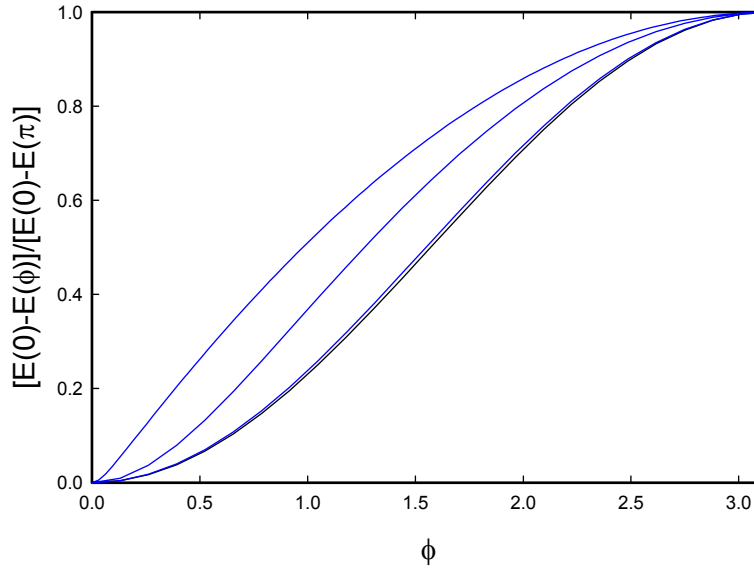
Figure 5. Relative self-energy as a function of phase angle ϕ for $\Delta n = 5$. Weak coupling limit is the lower curve in black; results from bottom to top in blue are for $g = 0.3, 1, 10$.

$$g_i = \frac{\sum_j H_{ij}}{\sum_j \Delta E}, \tag{34}$$

where the summation over j includes only states with non-zero coupling matrix elements from i. We plotted the self-energy for each state versus the approximate state g_i as points in Fig. 2, and we also plotted results for the self-energy as a function of g in the local approximation as a line. As can be seen, the agreement is excellent for all of the nearly-degenerate basis states.

5.4. Comparison of the indirect coupling matrix elements

In Fig. 3, we plotted the indirect matrix elements from each state as for each dimensionless coupling strength g_i as points, and results from the associated local approximation as a line. One sees good agreement for the larger values of g, which corresponds to the part of the problem where the different g_i values vary slowly (where we would expect the local approximation to be best). The agreement is not quite as good for the smaller g_i values. This is because the coupling matrix elements of the original Hamiltonian are most rapidly varying in this regime.

5.5. Discussion

We see from this comparison that the local approximation does very well in estimating the self-energy, which varies relatively slowly with g. The indirect coupling matrix element is a much stronger function of g, so the local approximation does not do quite as well. The underlying approximation that the coupling matrix elements of the original
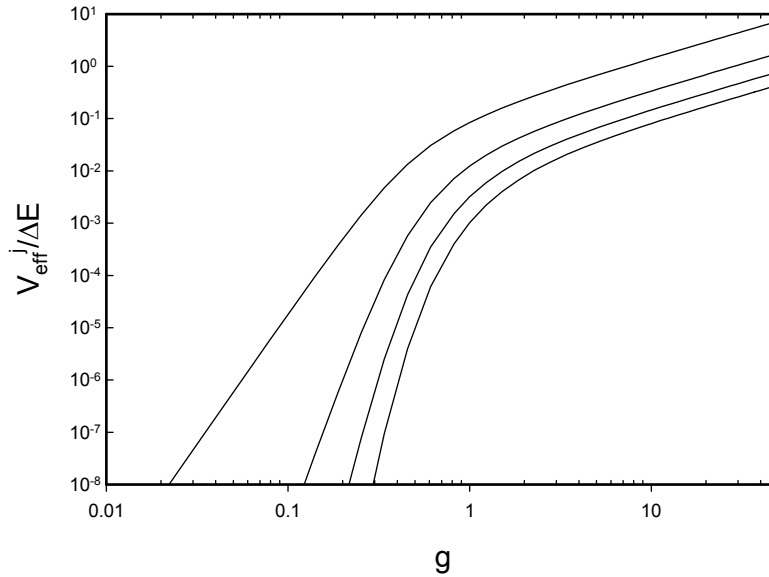
Figure 6.   Indirect coupling matrix elements between nearest neighbors (upper curve); second, third and fourth nearest neighbors (lower curves in descending order).

Hamiltonian are all the same begins to break down for small g. In this regime, the indirect matrix elements which couple to states where the local coupling is stronger becomes larger, while the indirect matrix elements which couple to states with weaker local coupling become smaller. In this regime, we see a splitting of the matrix elements for the two different directions (see Fig. 3). When this occurs, the indirect matrix elements from the local approximation lie between them.

In this model problem, the number of two-level systems is not particularly large. As a result, we end up seeing a weak departure between the numerically exact results from the second-order formulation and the results from the local approximation. In problems where the number of two-level systems is much larger, we would expect the local approximation to be much better, since the associated coupling matrix elements of the original problem generally will have smaller differences locally.

6. Local Approximation Results

One advantage of the local approximation is that we are able to carry out computations systematically for a wide range of dimensionless coupling constants g when the number of oscillator quanta exchanged is modest.

6.1. Self-energies

In Fig. 4, we show the self-energies as a function of g for the local approximation for different values of Δn. One sees that for larger values of Δn, the different self-energies quickly approach a large Δn limit. For small g the self energy is quadratic in g; and for large g the self-energy is linear in g.

6.2. Energy as a function of angle

We expect the self-energy to be dependent on the phase angle ϕ, with a simple sinusoidal dependence when the coupling is weak as discussed above. In Fig. 5, we show results for the relative self-energy in the case of five quantum exchange for different values of the dimensionless coupling constant g. When the coupling is very weak, nearest neighbor coupling is dominant, and

$$\frac{E(0) - E(\phi)}{E(0) - E(\pi)} \rightarrow 1 - \cos\phi. \tag{35}$$

We see that when $g = 0.3$ that the the relative self-energy is a good match, and that nearest neighbor coupling is dominant. For the larger values of the dimensionless coupling constant, there is some deviation from the cosine function, which indicates that coupling to second and higher neighbors contributes.

It is possible to extract from the angle-dependent self energy curves the coupling parameters for the different neighbors systematically. We have done this for the results shown in Fig. 5 to obtain the indirect coupling coefficients for the different neighbors in Fig. 6. From these results we see that nearest-neighbor coupling dominates, and that as the magnitude of the splitting gets larger the contributions from other neighbors increases.

6.3. Level splittings

Results for the normalized level splittings for different local approximation models as a function of g are shown in Fig. 7. In the event that the indirect coupling is weak, this normalized level splitting approaches the indirect coupling matrix element
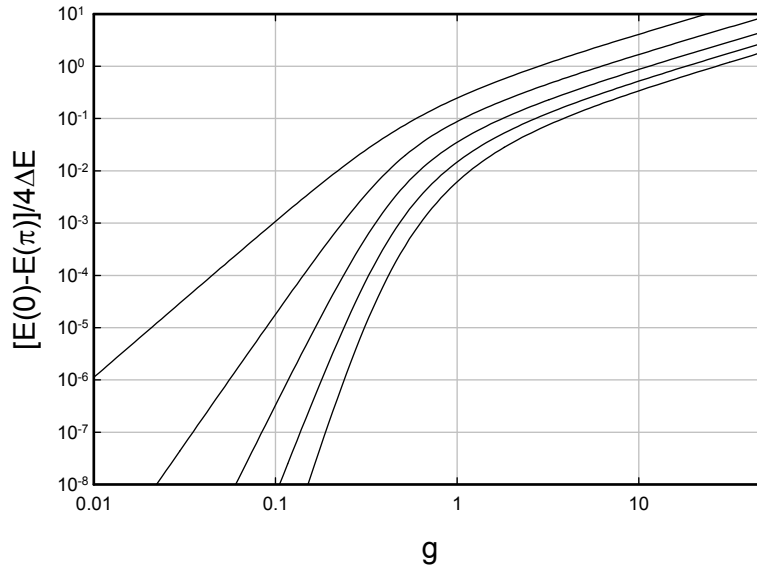

Figure 7.   Normalized level splitting as a function of g for $\Delta n = 3, 5, 7, 9, 11$ ($n = 3$ is the top curve, and $n = 11$ is the bottom).

$$\frac{E(0) - E(\pi)}{4} \; \rightarrow \; V_{\text{eff}} \tag{36}$$

It is easiest to carry out systematic computations for the level splitting, without isolating the contributions of indirect coupling between the different nearly degenerate neighbors.

In general, we see that the level splitting in the lossy spin-boson model decreases with the exchange of more oscillator quanta, and that the curves become sharper with a threshold at increasing g as Δn increases.

7. Discussion and Conclusions

In previous papers we have provided a systematic presentation of the lossy spin-boson model, which we have been interested in because of it is capable of fast coherent multi-quantum energy exchange between two-level systems and an oscillator. Although the model Hamiltonian is relatively simple in form, the analysis of coherent energy transfer between the two-level systems and the oscillator in the multi-quantum regime is not straightforward. In earlier work we have explored coherent energy exchange using perturbation theory, and a formulation that is based on a second-order Hamiltonian. Using these tools, we can study coherent energy exchange when a few quanta are exchanged under conditions where the coupling is weak to moderate. Here we introduced the local approximation, which greatly extends our ability to quantify coherent energy exchange in the model.

In the local approximation, we assume that the system is essentially unchanged when a single two-level system gains or loses excitation, such that the underlying coupling matrix elements do not change. The assumption leads to a problem that is periodic when the resonance condition is satisfied, and the resulting periodic problem is much easier to solve. We considered a model problem in order to see how good the local approximation does when compared to results obtained from the second-order Hamiltonian. The results from the local approximation were found to be very good under conditions where we would expect the local approximation to be good (large S, $S^2 - m^2 >> 0$).

Within the framework of the local approximation, we define a local value of the dimensionless coupling constant g, and the self-energy and indirect coupling matrix elements become unique functions of this g. We analyze the lossy spin-boson model in the limit of infinite loss, and the result of the analysis then is a determination of the associated self-energy and indirect matrix element functions versus g for a particular value of Δn. In practice, it is simpler to compute the level splitting $E(0) - E(\pi)$ than the indirect coupling matrix elements. This is useful since we know that nearest neighbor coupling dominates when the splitting is smaller than ΔE.

We have given results for the self-energy and level splitting for different values of Δn between 3 and 11 here. These results allow us to see the general trends that emerge. For example, the self-energy is quadratic at low g and linear when g is large. As the number of quanta exchanged becomes large, the self-energy curve approaches a large Δn limit. The level splitting (and coherent energy exchange rate) becomes smaller when more quanta are exchanged, as we might expect since intuitively we would expect the corresponding physical system to have more trouble breaking up a big quantum into smaller pieces.

What remains is for us to extend our analysis even further to understand what happens when Δn becomes large. From the results obtained so far, we would expect that g is going to have to become large in order to obtain a finite rate for coherent energy exchange. As we shall see, the local approximation presented in this paper is going to be of great help in analyzing this limit; however, we are going to need additional tools in order to extract quantitative results from the local approximation in this limit. (which we will discuss in a subsequent paper).

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