Research Article

Second-order Formulation and Scaling in the Lossy Spin-Boson Model

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Abstract

In the Fleischmann–Pons experiment, energy is produced without commensurate energetic reaction products. To account for this we have proposed new models in which coherent energy exchange occurs between two-level systems with a large energy quantum, and an oscillator with a much smaller characteristic energy. In earlier work we demonstrated using perturbation theory that the lossy spin-boson model is capable of efficient coherent energy exchange when many oscillator quanta are exchanged for a two-level system quanta on resonance. Here we introduce a formulation that isolates nearly degenerate states in the lossy spin-boson model, and allows the computation of the self-energy and indirect coupling matrix elements. From calculations of simple lossy spin boson models we establish a scaling law and define the dimensionless coupling constant g for the system. Direct calculations using this approach is not possible for large models in which a great many oscillator quanta are exchanged, but the formulation provides a foundation for understanding this kind of model, and will allow us to develop more powerful approximate methods.
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1. Introduction

We have been interested over the past decade or more in developing models [1–4] to account for excess heat in the Fleischmann–Pons experiment [5–8]. From our perspective, the key feature of these experiments which makes the development of a model difficult is the absence of energetic particles commensurate with the energy observed.

The only product which has been identified so far to be commensurate with the energy produced is ^{4}He, which is seen in the off-gas from the cathode [9–11]. We have used the results from experiment in which excess power is seen under conditions where an attempt was made to measure neutron emission in order to obtain an upper limit on the energy of the ^{4}He. We found that energetic alpha particles can collide with deuterons, resulting in secondary neutrons

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from subsequent deuteron–deuteron fusion reactions. The upper limit on the alpha energy estimated in this way is below 20 keV [12]. The experimental reaction energy per ^{4}He observed is close to 24 MeV [13].

These constraints tell us that no matter what process is responsible, it does not work in the same way as a Rutherford-type of reaction familiar in nuclear physics. Local conservation of energy and momentum in such reactions requires that the reaction energy must be expressed primarily as kinetic energy of the products. If two deuterons react to produce ^{4}He with most of the energy carried away by a gamma or electron, the resulting alpha particle would have an energy near 75 keV, which by itself is inconsistent with experiment (and there are no commensurate fast electrons or gammas observed).

This has motivated us to pursue new models in which the nuclear energy is transferred directly to low energy condensed matter degrees of freedom, such as vibrational modes [1–4]. There is no precedence for this in nuclear physics or condensed matter physics. Coherent many quantum exchange between an oscillator and two-level systems is known in NMR and in problems involving atomic states and an electromagnetic field [14–16]. However, in these models, the number of quanta exchanged is less than 10^2, where on the order of 10^8 would be required to account for the Fleischmann–Pons experiment.

Some years ago, we found new models which are much more efficient at exchanging a large number of quanta [1]. In two recent papers, we began a program of laying out the new models systematically. In the first, we introduced the lossy spin-boson model more properly than in earlier work, we reviewed the sector formalism that underlies loss in a second-order Hamiltonian, and we showed that coherent energy exchange is enhanced dramatically using lowest-order perturbation theory [17]. In the second, we considered the dynamics of a set of nearly degenerate states that have nearest neighbor coupling, and developed reasonably general evolution formula for the dynamics of number and velocity expectation values [18].

Here, we extend the discussion to a second-order formulation which isolates the nearly degenerate states. In previous work on the (lossless) spin-boson model, we studied a rotation which isolated the nearly degenerate states, and allowed us to model the indirect coupling between them simply [19,20]. We have not found an analogous rotation for the lossy version of the problem, but the second-order formulation accomplishes a similar function.

Perhaps the biggest advantage of this formulation is that it allows us to reduce a complicated problem (the lossy spin-boson model) into a much simpler one (a set of nearly degenerate states where the nearest neighbor coupling is dominant). We can use this formulation to compute the self-energies of the nearly degenerate states (which can remove the approximate degeneracy when the coupling is strong), and also the indirect coupling matrix elements. In the latter case, we can compare with perturbation theory in order to verify that the approach is correct in the weak coupling limit. We are able to use this approach to begin to understand how scaling works in the lossy spin-boson model, and to define a relevant dimensionless coupling coefficient.

A disadvantage of the approach is that the matrix calculations that result do not scale well as the number of states increase. So, if we focus on models that involve the exchange of only a few quanta (three, five, or seven), then we can perform calculations effectively even when the coupling is beginning to be strong. However, if we attempt computations for models with tens or hundreds of quanta exchanged, this approach is too slow to give us results in a reasonable time.

Even though the second-order formulation is not capable of handling the problems that we are ultimately interested in, it does provide us with a foundation that we can use for the development of approximation schemes which greatly extend our ability to analyze these models. A discussion of these approximation schemes is deferred to a following paper.

2. Coupling Between Nearly Degenerate States

We begin with the lossy spin-boson model, which is described by the Hamiltonian [17]

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

Here ΔE is the transition energy between the two-level systems, $\hbar\omega_0$ is the characteristic energy of the oscillator, and V describes the strength of the interaction. We have used many-spin operators $\hat{S}_z$ and $\hat{S}_x$ to describe the two-level systems. The model assumes identical two-level systems with identical linear interactions with the oscillator.

Loss is included using a Brillouin–Wigner formulation as we have reviewed previously [17]. In the case of a general loss model, the model that results is very complicated, and it becomes difficult to analyze. In this paper we will make an assumption about the loss in order to simplify things. In the infinite loss version of the model, we would assume that the loss is infinitely fast (resulting in zero occupation of the lossy states) when the basis state energy is less than E. Although this drastically reduces the complexity of the model, we find that even this simplified version of the model has technical issues associated with it due to the self-energy when the coupling is not weak. Instead, our focus will be on the closely related fixed basis version of the model, where we exclude all basis states with an energy less than the basis state energy of the nearly degenerate set initially selected.

2.1. Nearly degenerate states

We expand in terms of two sets of basis states

$$\Psi \;=\; \sum_j c_j \Phi_j^a + \sum_k d_k \Phi_k^b, \tag{2}$$

where the Φ_j^a states are of the form

$$|S, m\rangle |n\rangle, \quad |S, m-1\rangle |n + \Delta n\rangle, \quad \ldots,$$

which are nearly degenerate at the energy E of interest. Here Δn is the number of oscillator quanta exchanged per unit change in the excitation of the two-level systems. The Φ_k^b states include all of the other basis states with higher energy.

2.2. Isolation of the nearly degenerate states

Our goal is the development of a formulation that allows us to describe the slow evolution of the system between the nearly degenerate states. To accomplish this, we would like to focus on the c_j expansion coefficients of the degenerate basis states, and eliminate the other coefficients. To proceed, we start with the algebraic eigenvalue coefficients for the two sets of expansion coefficients (which we write in vector and matrix form)

$$E\mathbf{c} \;=\; \mathbf{H}_a \cdot \mathbf{c} + \mathbf{V}_{ab} \cdot \mathbf{d},$$

$$E\mathbf{d} \;=\; \mathbf{H}_b \cdot \mathbf{d} + \mathbf{V}_{ba} \cdot \mathbf{c}. \tag{3}$$

Since the b states are not degenerate at energy E, we can write the $\mathbf{d}$ vector in terms of the $\mathbf{c}$ vector as

$$\mathbf{d} \ = \ (E - \mathbf{H}_b)^{-1} \cdot (\mathbf{V}_{ba} \cdot \mathbf{c}). \tag{4}$$

This allows us to obtain a reduced implicit eigenvalue problem

$$E\mathbf{c} \ = \ \mathbf{H}_a \cdot \mathbf{c} + \mathbf{V}_{ab} \cdot (E - \mathbf{H}_b)^{-1} \cdot \mathbf{V}_{ba} \cdot \mathbf{c}. \tag{5}$$

2.3. Hamiltonian matrix for the nearly degenerate states

The associated second-order Hamiltonian matrix can be written as

$$\mathbf{H}(E) \ = \ \mathbf{H}_a + \mathbf{V}_{ab} \cdot (E - \mathbf{H}_b)^{-1} \cdot \mathbf{V}_{ba}. \tag{6}$$

This new second-order matrix $\mathbf{H}(E)$ is much smaller than the total matrix made up of $\mathbf{H}_a$, $\mathbf{H}_b$, $\mathbf{V}_{ab}$, and $\mathbf{V}_{ba}$, and we can use it for computations specifically on the c_j coefficients. Since the energy eigenvalue appears explicitly in the denominator, this Hamiltonian matrix is more complicated to work with than more standard Hamiltonians. Nevertheless, we can use iterative numerical methods to achieve self-consistency between a specific eigenvalue and the eigenvalue in the denominator.

3. Three-phonon Exchange and Scaling

One of our goals is the demonstration of a scaling law for the lossy spin-boson model. It seem reasonable to make use of the formulation outlined in the previous section to explore scaling for a specific example. The simplest example which shows enhanced coupling between nearly degenerate states is a problem in which a single two-level system quantum is matched to three oscillator quanta

$$\Delta E \ = \ 3\hbar\omega_0. \tag{7}$$

Since the numerical computations outlined increase rapidly when there are a very large number of states involved, we can minimize the number of states for a set of computations by reducing the number of oscillator quanta that are exchanged.

The notion of scaling is familiar to those working on various physics models, such as the spin-boson problem. If we were writing for those working on the this problem, probably a single line and scaling formula would suffice. However, the intended audience for this paper includes researchers who may not be familiar with the idea in the context of this kind of model. As a result, we are interested in clarifying the issue through the examination of a set of specific calculations.

3.1. Energy levels and scaling

The simplest way to understand what a scaling law does is by considering solutions for different examples which satisfy the scaling law. We consider two solutions with different numbers of two-level systems, under conditions where the maximum off-diagonal coupling matrix element for the original lossy spin-boson model are the same.

The largest matrix element has a magnitude of approximately

$$\max\{\langle S, m, n|\hat{H}|S, m \pm 1, n \pm 1\rangle\} \ = \ V\sqrt{n}S. \tag{8}$$
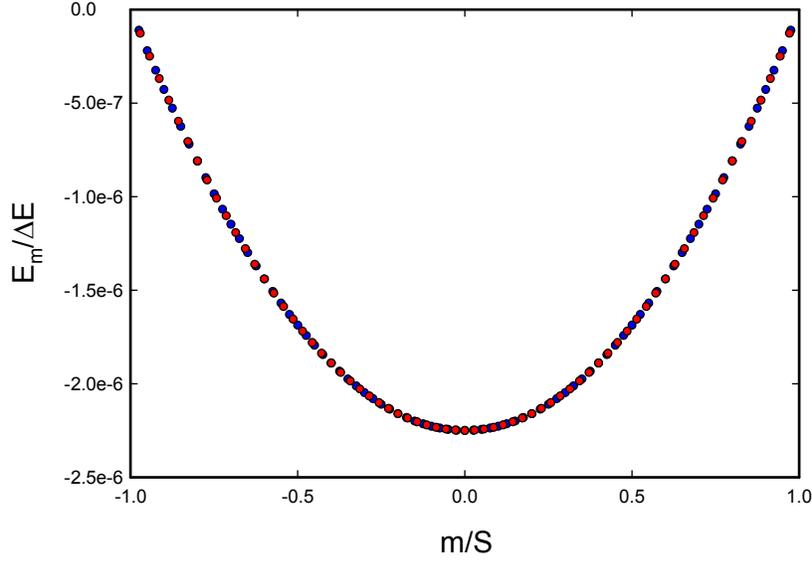
Figure 1.   Reduced basis energies for 69 (red) and 79 (blue) two-level systems.

In Fig. 1, we show results for the diagonal matrix elements for $\mathbf{H}(E)$ in the case of 69 ($S = 34$) and 79 ($S = 39$) two-level systems. The product $V\sqrt{n}S$ is the same ($9.75 \times 10^{-3}\ \Delta E$) in both calculations. We have taken $n = 10^{12}$, and used different values for V to match the largest matrix element. We see that the diagonal energies line up together when plotted this way.

### 3.2. Dimensionless coupling strength

It is customary to define a dimensionless coupling strength g for this kind of problem. In this case, we would take the ratio of the magnitude of the coupling matrix element to the two-level transition energy, so that the maximum coupling strength is

$$\max\{g\} \;=\; \frac{V\sqrt{n}S}{\Delta E}. \tag{9}$$

The intuition that we seek to develop in what follows is that the local dimensionless coupling strength g determines the important parameters of the model, such as the self-energy and the indirect coupling matrix element between nearest neighbors.

3.3. Indirect coupling matrix elements

The indirect coupling matrix elements between nearest nearly degenerate neighbors are shown in Fig. 2 for the same calculations as for Fig. 1. We can make use of perturbation theory to compute the effective coupling matrix element for a transition from $|n, S, m\rangle$ to $|n - 3, S, m + 1\rangle$, which leads to
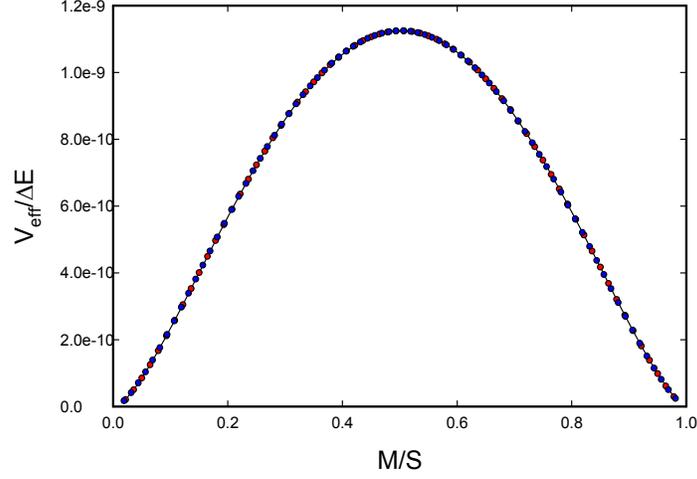
Figure 2.   Indirect matrix element between nearly degenerate states for 69 (red) and 79 (blue) two-level systems.

$$V_{eff} \; = \; \frac{9}{8} \frac{V^3}{\Delta E^2} (S^2 + S - m^2 - 3m - 2) \sqrt{S^2 + S - m^2 - m} \sqrt{n(n-1)(n-2)}. \tag{10}$$

This perturbation theory result is indicated as a solid black line in Fig. 2. The two different problems that we have examined give very similar results for the indirect coupling matrix elements, and these results are in good agreement with the results from perturbation theory.

3.4. Decoupling of one basis state

One of the nearly degenerate states is decoupled from the others in this model. Consider the basis state

$$\Phi \; = \; |S, S, n_0\rangle. \tag{11}$$

in which all of the two-level systems are excited, and in which there are no excess oscillator quanta. This state has non-vanishing coupling matrix elements only to

$$|S, S - 1, n_0 \pm 1\rangle. \tag{12}$$

The energy of these states is below the cut-off energy in this model. Such states are presumed to be very lossy, and hence have a zero occupation probability in the infinite loss model. If so, then $|S, S, n_0\rangle$ becomes decoupled from the other states.

In Fig. 3, we show the lowest loss path in this case in a perturbation theory scheme. Two of the intermediate states have basis energies that are lower than that of the initial state, and which can decay. For comparison, we show the
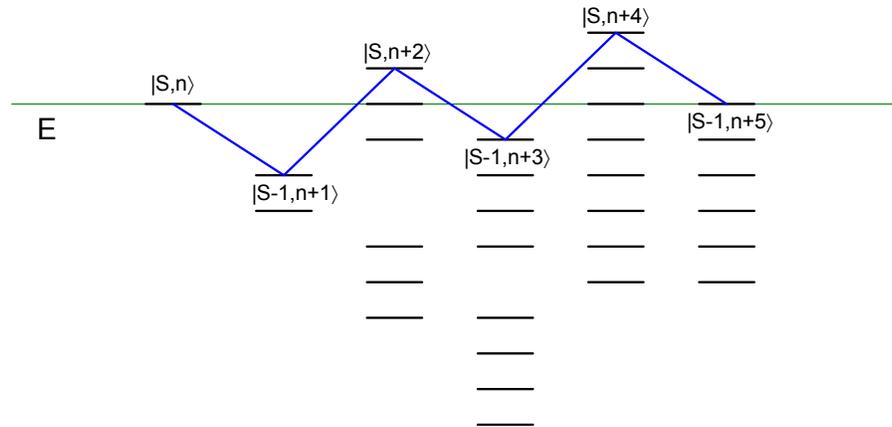
Figure 3. Levels and transitions for lowest loss pathway in perturbation theory starting from $|S, S, n\rangle = |S, n\rangle$, in the case of $\Delta E = 5\hbar\omega_0$.

lowest loss path in the general case in Fig. 4. In this case, none of the intermediate states have basis energies below that of the initial state, so that decay processes are minimized.

Coupling from this state in finite loss models would by necessity involve coupling through a lossy intermediate state. This is the first time in the present discussion that we come across this issue. When we consider more complicated models in papers that follow, we will find that this effect occurs generally in models of interest to us. We will eventually connect this effect with the low-level emission of energetic particles that is seen in some Fleischmann–Pons experiments.

3.5. Discussion

The specific problem that we selected to focus on in this section appears now to be very simple to understand. The second-order Hamiltonian leads to basis state energies that are very close to parabolic in m under conditions where perturbation theory is valid. The coupling between neighboring nearly degenerate states is dominant, and closely matches the result from perturbation theory.

In order for the associated system to exchange energy between the two degrees of freedom efficiently, all that we need is for the coupling matrix element between neighboring states to be as large as the splitting between neighboring states or greater. In this model, it seems clear how to do it. The more two-level systems that we have, the smaller the interaction we choose (in the scaling outlined above), so the smaller the difference between neighboring states. The coupling between neighboring states is strongest when about half of the two-level systems are excited, and is approximately constant with the number of two-level systems when scaled as above. Hence, as there are more two-level systems, we are able to maintain coherence over a larger fraction of the Dicke states.
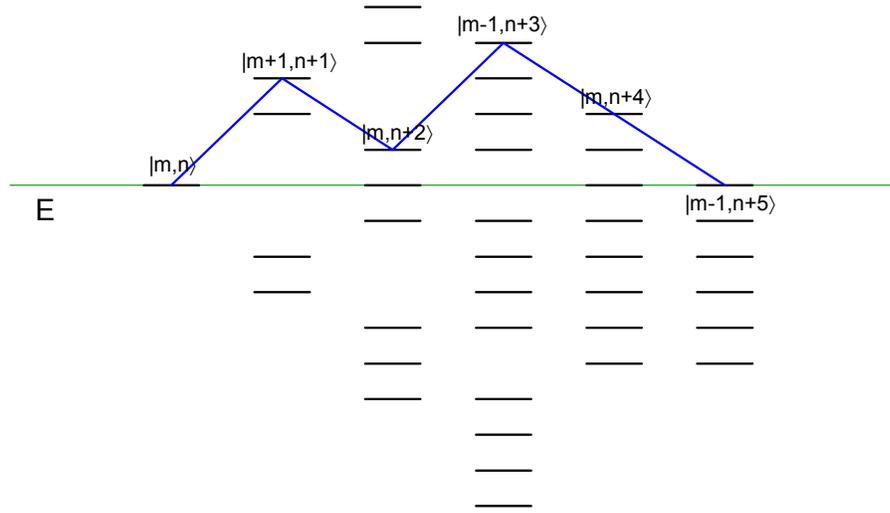
Figure 4. Levels and transitions for lowest loss pathway in perturbation theory starting from $|S, m, n\rangle = |m, n\rangle$, in the case of $\Delta E = 5\hbar\omega_0$.

4. Practical Issues

The isolation of a set of nearly degenerate states as outlined above is a very useful way to think about the problem, and provides a way to compute the important parameters of the model. However, as we start to go further in this direction, new issues arise. There is a practical computational issue concerning how to determine the energy eigenvalue self-consistently, since it appears in the second-order Hamiltonian. The self-energy shift tends to split the nearly degenerate states, so that we would like to understand under what conditions energy exchange can occur. The self-energy shift in addition impacts our selection of basis states, which motivates us to consider a restricted basis approximation.

4.1. Solving the second-order eigenvalue problem

If the dimensionless coupling strength is small, then the self-energy is also small, which means that one can obtain solutions to the second-order eigenvalue equation

$$E\mathbf{c} = \mathbf{H}_a \cdot \mathbf{c} + \mathbf{V}_{ab} \cdot (E - \mathbf{H}_b)^{-1} \cdot \mathbf{V}_{ba} \cdot \mathbf{c} \tag{13}$$

by using the unperturbed basis state energy on the right hand side. When the self-energy begins to become significant, then the accuracy of the energy eigenvalues computed this way is degraded. We can obtain accurate results by solving for the energy eigenvalue self-consistently, as discussed in Appendix B.

Unfortunately, it quickly becomes inconvenient to obtain numerical solutions using this approach as the number of quanta exchanged becomes larger, and when the dimensionless coupling strength is near or above unity. This will motivate us to pursue an approximate solution to the problem, which we will consider below.

4.2. Constraint for maintaining coherence

From the results in the previous section, we have seen that models with the same maximum dimensionless coupling coefficient g are very similar in terms of their self-energy and indirect coupling matrix elements. We can think of a family of models where the maximum dimensionless coupling constant is held fixed, and the number of two-level systems is varied (assuming that n is kept constant and large). For this family of models, the self-energy and indirect coupling matrix elements as a function of M/S are nearly the same. However, if the states were initially degenerate, then the splitting of the states is reduced when we have more two-level systems.

When we considered the dynamics resulting from the coupling between nearly degenerate states, we found that the problem was simplest in the case of degenerate basis states. If there is a splitting between the states, then this can alter the dynamics. In order for energy exchange to proceed at rates close to that for the degenerate version of the problem, we require that the splitting be less that the indirect coupling

$$|E_{m+1} - E_m| \; < \; |V_{m+\frac{1}{2}}| \tag{14}$$

in the notation of the previous paper. If the basis states are initially degenerate, then the splitting of interest for this constraint will be due to the self-energy shift. In this case, as we increase the number of two-level systems, the splitting will decrease, and more of the nearly degenerate states will be able to participate in the dynamics.

4.3. Constraint for three-quantum exchange

We can develop an approximate version of the constraint in the special case of three quantum exchange that we discussed above. The self-energy shift for small g is approximately

$$E_m \; = \; -0.0237 \, (\max\{g\})^2 \left[1 - \left(\frac{m}{S} \right)^2 \right] \Delta E \tag{15}$$

so that

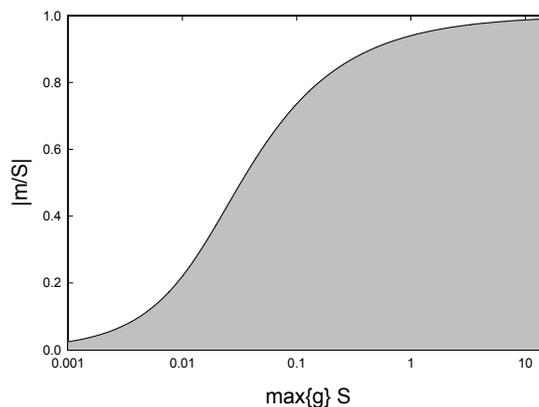$$|E_{m+1} - E_m| \; = \; 0.0237 \, (\max\{g\})^2 \left(\frac{2|m|}{S^2} \right) \Delta E. \tag{16}$$

The matrix element for indirect coupling from perturbation theory is approximately

$$V_{\text{eff}} \; = \; \frac{9}{8} (\max\{g\})^3 \left[1 - \left(\frac{m}{S} \right)^2 \right]^{3/2} \Delta E \tag{17}$$

in the limit that S and n are large. We can combine these estimates to obtain

$$\frac{\left| \dfrac{m}{S} \right|}{\left[1 - \left(\dfrac{m}{S} \right)^2 \right]^{3/2}} \; < \; 23.7 \, \max\{g\} S. \tag{18}$$

This constraint is illustrated in Fig. 5.

Figure 5. Evaluation of the constraint (18) in the case of three quantum exchange. The region in gray is where the level splitting is less than the indirect coupling matrix element.

4.4. Self-energy as potential energy of the coupled system

When the self-energy becomes large, there can be a significant shift of the energy levels. For example, when the coupling is near unity, the self-energy can be on the order of ΔE. Since this self-energy seems to be large, we need to think some about what it means, and what the implications are for our approximation.

The self-energy comes about due to the interactions in the model that produces the coupling between the states. Perhaps it is best to think of it as a binding energy or equivalently, a potential energy, for the coupled systems. If so, then it may be best to think of it on a per two-level system basis, especially if n is very large. For large g the self-energy becomes linear in g, so that this point of view will be helpful much later on when we consider models which seek to describe the Fleischmann–Pons excess power effect. Under the conditions that we have encountered so far, this self-energy per two-level system is small compared to the transition energy ΔE. It can be substantial compared to the oscillator energy, especially when a large number of oscillator quanta are exchanged.

4.5. Fixed basis state model

In the lossy spin-boson model with infinite loss, we proposed that all states with an energy less than E were to be assumed to have infinite loss. If the self-energy is small, then the basis state energy will not be so different from the diagonal energy in the second-order $\mathbf{H}(E)$ matrix. Hence, in this limit the choice of which states to keep and which to omit is clear.

However, if we include the self-energy, then things become more complicated. If we omit all states with an energy less than some energy E, and then calculate the diagonal energies for the $\mathbf{H}(E)$ matrix, we will find that many of the resulting states have an energy less than the energy E which we selected as a cut-off due to the contribution of the self-energy. If the dimensionless coupling constant g is close to unity, this contribution can be very large.

One approach to this problem is to go back and revise the list of included and omitted states so as to be self consistent with a cut-off energy. Another approach to the problem is to fix the basis initially, and keep it throughout the calculation. This latter approach is much more convenient for numerical calculations. In the limit that there are many oscillator quanta exchanged for each two-level transition, then this kind of model will lead to minor errors locally in the list of
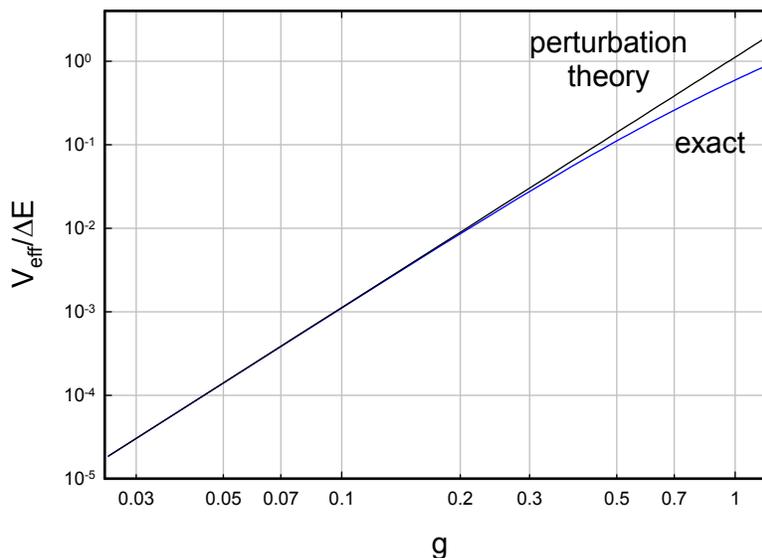
Figure 6. Largest normalized effective indirect coupling matrix element $V_{\mathrm{eff}}/\Delta E$ as a function of g computed using $S = 19$ (blue); perturbation theory result (black). The number of oscillator quanta used in this calculation is 10^{12}.

states that are retained (it will keep too many). We would not expect this to lead to significant changes in the model parameters or dynamics, but we have not pursued this issue in our work.

In Fig. 6, we show results from such a computation for the largest indirect coupling matrix element as a function of g. In most of the calculations that will follow in this and in following papers, we will work with this kind of model.

5. Discussion and Conclusions

In a previous paper of this set [17], we introduced the lossy spin-boson model and showed that it was capable of greatly enhanced coherent energy exchange (as compared to the lossless spin-boson model) when many oscillator quanta are exchanged for a two-level system quantum. In this we are pleased that the new model is capable of such efficient coherent energy exchange, since it is the basic effect that in our view is needed to account for excess heat in the Fleischmann–Pons experiment.

However, it is clear that we are going to need much stronger analytical tools to obtain results in a relevant regime. Perturbation theory is helpful when the coupling is weak, but we are going to need the model to work in a very strong coupling limit in order to convert a single two-level system quantum into 10^8 oscillator quanta. As a result, we need to develop models and approximations which are useful in the strong coupling limit.

The second-order formulation that we introduced above allows us to extend our modeling well beyond the weak coupling limit. We can use it directly to analyze the lossy spin-boson model when a relatively small number of oscillator quanta are exchanged. This is useful since it allows us to discuss scaling for this model, and also to introduce the dimensionless coupling constant g.

We cannot use the second-order formulation presented here for direct calculations of models in which millions of

quanta are exchanged for each two-level system transition, since the approach does not scale well as a computational problem. What is important here is the notion that we can isolate the nearly degenerate states, and that the self-energy and the matrix elements for indirect coupling between nearest neighbors obey scaling laws. For example, even though we are not able to perform a computation with 10^{10} two-level systems, we would have no trouble developing accurate estimates for the self-energy and indirect coupling between nearest neighbors for weak and moderately strong coupling in the case of 3 or 5 quantum exchange because of the scaling law. We still need to develop a scaling law that governs the self-energy and indirect coupling matrix element in the limit where a large number of oscillator quanta are exchanged.

In a paper that follows, we will present an approximation scheme which is based on the formulation presented here that will allow us to perform calculations for models where a much larger number of oscillator quanta are exchanged. Based on these results we will be able to deduce a scaling law that is useful generally when the number of oscillator quanta exchanged is large.

Appendix A. Numerical issues

The algebraic problem as outlined in Section 2 seems completely straightforward, but there are significant issues that remain. Some of these concern numerical issues which we must face when implementing the approximation. We will provide a brief discussion of a simple numerical approach in the subsections that follow.

Appendix A.1. Selection of basis states

We first consider the selection of basis states. We have the parity selection rule that states with positive parity $(-1)^{n+m}$ do not couple with states with negative $(-1)^{n+m}$. So, we have chosen to work with positive parity states here.

Next, we note that the number of Dicke states associated with the two-level systems alone is $2S + 1$, since all of the two-level systems can be in the ground state ($m = -S$) and all of them can be in the excited state ($m = S$). The line for equal energy is defined according to

$$E = \Delta E m + \hbar \omega_0 n. \tag{A.1}$$

It seems reasonable to keep states up to some fixed energy above the threshold energy, which we define here has being

$$E_0 = \Delta E S + \hbar \omega_0 n_0. \tag{A.2}$$

At this energy, all of the two-level systems are excited, and the oscillator has nominal excitation n_0.

Appendix A.2. Banded Cholesky decomposition

In the algebraic equation above, we need to compute the inverse of a matrix. While this seems straightforward, not all numerical algorithms will result in a symmetric inverse. Consequently, we need to pay some attention to how this is carried out.

To proceed, we define

$$\mathbf{A} = \mathbf{A}(E) = \mathbf{H}_b - E. \tag{A.3}$$

Since $\mathbf{A}$ is symmetric, LU decomposition can be carried out using

$$\mathbf{A} \;=\; \mathbf{L} \cdot \mathbf{L}^{\mathrm{T}}, \tag{A.4}$$

where $\mathbf{L}$ is lower triangular.

We can use Cholesky decomposition in order to decompose $\mathbf{A}$. This algorithm seems to work pretty well for this problem. We are aided by the fact that $\mathbf{A}$ is banded, which speeds the computation of $\mathbf{L}$, and leads to a banded matrix $\mathbf{L}$. Even for a very large problem, we are able to compute $\mathbf{L}$ by Cholesky decomposition conveniently.

Appendix A.3. Matrix inverse of the lower triangular matrix

For the solution linear systems, Cholesky decomposition is the time-consuming part of the algorithm in the case of symmetric matrices. Determination of the solution is done by back substitution. We have tried various algorithms based on back substitution, however, it seemed useful along the way to carry out an explicit construction of the inverse, and we subsequently kept it.

The construction of the inverse of a lower triangular matrix can be done reasonably efficiently in the case of a banded matrix. The algorithm that we have used works as follows. We assume that the inverse is also a lower triangular matrix $\mathbf{B}$, so that

$$\mathbf{B} \cdot \mathbf{L} \;=\; \mathbf{I}. \tag{A.5}$$

To understand the associated algorithm for determining $\mathbf{B}$, it is useful to write this equation out explicitly in the case of 3×3 matrices. We may write

$$
\begin{pmatrix} B_{11} & 0 & 0 \\ B_{21} & B_{22} & 0 \\ B_{31} & B_{32} & B_{33} \end{pmatrix} \cdot \begin{pmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{pmatrix} =
$$
$$
\begin{pmatrix} B_{11}L_{11} & 0 & 0 \\ B_{21}L_{11}+B_{22}L_{21} & B_{22}L_{22} & 0 \\ B_{31}L_{11}+B_{32}L21+B_{33}L_{31} & B_{32}L_{22}+B_{33}L_{32} & B_{33}L_{33} \end{pmatrix}. \tag{A.6}
$$

It seems clear that we can solve for diagonal terms directly using

$$B_{ii} \;=\; \frac{1}{L_{ii}}. \tag{A.7}$$

If we go off of the diagonal by one, we end up with equations of the form

$$B_{i,i-1}L_{i-1,i-1} + B_{ii}L_{i,i-1} \;=\; 0. \tag{A.8}$$

We can solve this using

$$B_{i,i-1} \;=\; -\frac{B_{ii}L_{i,i-1}}{L_{i-1,i-1}}. \tag{A.9}$$

It is possible to continue the algorithm to determine the different B_{ij} values based on a knowledge of known L and previously determined B matrix elements.

Appendix A.4. Construction of the second-order matrix

The second-order matrix can be written as

$$\mathbf{H}(E) \;=\; \mathbf{H}_a - \mathbf{V}_{ab} \cdot \mathbf{A}^{-1}(E) \cdot \mathbf{V}_{ba}. \tag{A.10}$$

This can be written in terms of $\mathbf{L}$ as

$$\mathbf{H}(E) \;=\; \mathbf{H}_a - \mathbf{V}_{ab} \cdot (\mathbf{L} \cdot \mathbf{L}^{\mathrm{T}})^{-1} \cdot \mathbf{V}_{ba} \;=\; \mathbf{H}_a - \mathbf{V}_{ab} \cdot (\mathbf{L}^{\mathrm{T}})^{-1} \cdot \mathbf{L}^{-1} \cdot \mathbf{V}_{ba}. \tag{A.11}$$

We can recast this as

$$\mathbf{H}(E) \;=\; \mathbf{H}_a - (\mathbf{L}^{-1} \cdot \mathbf{V}_{ba})^{\mathrm{T}} \cdot (\mathbf{L}^{-1} \cdot \mathbf{V}_{ba}). \tag{A.12}$$

In this form, the resulting second-order matrix is explicitly real and symmetric, which was one of the goals of our construction.

Appendix B. Self-consistent computation of the energy

The Schrödinger equation in the case of the second-order Hamiltonian can be written as

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

We see that the energy eigenvalue appears both on the right-hand side (RHS) and on the left-hand side (LHS) of this equation. If the self-energy shift is small, then we can approximate the energy on the RHS with the basis state energy and obtain good results. If the self-energy shift is large, then a self-consistent calculation is needed.

Appendix B.1. Simple iteration

Iterative schemes can be used to obtain a self-consistent solution. The simplest iterative scheme can be written as

$$E^{(k+1)}\mathbf{c} \;=\; \mathbf{H}_a \cdot \mathbf{c} + \mathbf{V}_{ab} \cdot (E_j^{(k)} - \mathbf{H}_b)^{-1} \cdot \mathbf{V}_{ba} \cdot \mathbf{c}. \tag{B.2}$$

On the LHS, we have the energy eigenvalue in general $E^{(k+1)}$ for the $k+1$ iteration; on the RHS we have one particular basis state energy E_j^k determined on the previous iteration. If the scheme converges, then it can be stopped when the change in the energy eigenvalue of the state of interest doesn't change any more

$$|E_j^{(k+1)} - E_j^{(k)}| \;<\; \epsilon. \tag{B.3}$$

The iterations can be started by taking the initial energy equal to the initial basis state energy.

Appendix B.2. Iterations with relaxation

We have found that the iterations described above do not converge when the dimensionless coupling coefficient approaches unity. In this case, we have been able to converge using a modification of the scheme with relaxation based on

$$E^{(k+1)}\mathbf{c} \;=\; \mathbf{H}_a \cdot \mathbf{c} + \mathbf{V}_{ab} \cdot (F_j^{(k)} - \mathbf{H}_b)^{-1} \cdot \mathbf{V}_{ba} \cdot \mathbf{c}, \tag{B.4}$$

where

$$F_j^{(k)} \;=\; a E_j^{(k)} + (1-a) E_j^{(k-1)} \tag{B.5}$$

with a taken to be near 0.2.

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