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## **Models relevant to excess heat production in Fleischmann-Pons experiments**

**Peter L. Hagelstein and Irfan U. Chaudhary**

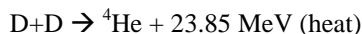
**Research Laboratory of Electronics, Massachusetts Institute  
of Technology, Cambridge, MA 02139 USA,  
plh@mit.edu**

Observations of excess heat in the absence of commensurate energetic charged particles challenges local energy and momentum conservation, a foundation of nuclear physics. We have explored models based on excitation transfer, in which global energy is conserved but local energy conservation is violated. We present recent results on both excitation transfer and anomalous energy exchange within the context of lossless spin-boson models. We introduce a rotation that allows us to isolate terms in the rotated Hamiltonian responsible for both processes. Spin-boson type models augmented with loss appear to be sufficiently strong to account for the excess heat effect.

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Claims of excess heat production in the Fleischmann-Pons experiment [1-3] were met with disbelief following the initial announcement of the effect in 1989 [4]. In the controversy that followed, discussions centered on experimental questions of reproducibility, calorimetry, absence of energetic products correlated with the energy, and the initial lack of identification of an ash quantitatively correlated with the energy production. Discussions centered also on theoretical issues, such as the low associated reaction rates expected for conventional deuteron-deuteron fusion reactions due to the Coulomb barrier, competition with the primary  $n+{}^3\text{He}$  and  $p+t$  reaction channels, and on the seeming impossibility of coupling the MeV-scale nuclear reaction energy to low-energy atomic degrees of freedom associated with the solid state environment.

Research over the subsequent 18 years has clarified some of these issues. Several groups have reported good reproducibility in experiments with excess heat; similar positive results have been reported with very different calorimeters; and  ${}^4\text{He}$  has been detected in amounts commensurate with the excess energy produced (see Ref. [5] and references therein). In the latter case, the reaction energy determined experimentally appears to be 24 MeV, suggesting an overall reaction mechanism consistent with



We recognize the existence of the conventional version of this reaction channel with  ${}^4\text{He}$  and an energetic gamma in the exit channel; however, there is no evidence for energetic gammas being produced in amounts commensurate with the energy production in any Fleischmann-Pons experiment. In essence, excess heat in the Fleischmann-Pons experiment requires the existence of a new physical process, since no known nuclear reaction works this way.

The reaction energy from a conventional nuclear reaction, and in particular from a fusion reaction, is expressed through energetic particles as a consequence of local energy and momentum conservation. Local energy and momentum conservation has been a foundation of nuclear physics since the time of Rutherford [6], and one can find relevant expositions in modern nuclear physics texts [7]. Excess heat production in the Fleischmann-Pons experiment challenges this foundation. Nuclear physicists since 1989 have been enthusiastic neither about either the Fleischmann-Pons experiment, nor about any discussion that includes a consideration of nuclear energy production in the absence of observations of energetic particles. No nuclear physics experiment within the entire nuclear physics literature dating back to before 1900 is thought to work this way; which leads to the tentative conclusion that this is because no nuclear reaction can produce energy without energetic particles.

Such a position was adopted in the 1989 ERAB report [8], and by Huizenga in his book [4]. Until proven otherwise independent of the Fleischmann-Pons experiment, it is unlikely that the situation will change.

All of which provides motivation for the models discussed below. We have focused for several years on a class of models, which seek to address violations of local energy and momentum conservation, and also to address the problem of the conversion of a large energy quantum into a large number of smaller energy quanta [9-11]. We view these two issues as separate problems, as will become clearer in the models themselves.

We take advantage of a quantum excitation transfer effect in order to violate local energy conservation, while preserving overall energy conservation. For example, if two deuterons react to form  ${}^4\text{He}$  in such a model, the reaction energy is transferred elsewhere, so that there is no need for energetic particles from the initial four-nucleon system. Once this excitation transfer has occurred, we still need to convert the large MeV energy quantum into a very large number of atomic scale quanta. The basic mechanism under consideration for this is one in which the excitation is transferred one small energy quantum at a time in a very large number of interactions, including fast excitation transfer reactions to other nuclei, and self interactions.

These notions already imply a set of models that can be studied, and we present below some results from our analysis of these systems. The results are interesting in the sense that we can establish an excitation transfer effect, as well as an energy exchange effect (in which a large quantum is split into a large number of small quanta), using very simple models composed of equivalent two-level systems and an oscillator. We would expect such models to fall short of describing the real system because they do not include loss effects. When we augment such models to include loss, we find that the excitation transfer and energy exchange effects become much stronger. Hence, models composed of two-level systems and an oscillator that are augmented with loss, appear to be candidates to describe the excess heat effect in Fleischmann-Pons experiments.

## Anomalous Energy Exchange

We consider first the anomalous energy exchange effect. We consider a two-level system with a large transition energy  $\Delta E$  coupled to a simple harmonic oscillator with a small characteristic energy  $\hbar\omega_0$ , with linear coupling. Our focus is on the rate at which energy is exchanged between the two systems. For this model, we adopt a spin-boson Hamiltonian given by

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

In writing this Hamiltonian, we use pseudospin operators  $\hat{s}_z$  and  $\hat{s}_x$  to describe the two-level system, and creation and annihilation operators for the simple harmonic oscillator. The coupling between the two systems has an interaction strength  $V$ . Models of this kind have been considered in the literature since the early work of Bloch and Siegert [12]. Models for the energy shifts and resonance conditions for this problem have been discussed in the literature over the years (see [13-17]).

A direct computation of energy levels from this Hamiltonian leads to an empirical parameterization of the energy levels according to

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

where the dressed two-level system energy  $\Delta E(g)$  depends on the interaction strength and on the number of oscillator quanta through the dimensionless coupling strength  $g$ , which we define according to

$$g = \frac{V\sqrt{n}}{\Delta E} \quad (3)$$

The relation between  $\Delta E(g)$  and  $g$  is roughly

$$\Delta E(g) = \sqrt{1 + 8g^2} \Delta E \quad (4)$$

as illustrated in Figure 1. One sees that this empirical parameterization is in reasonable agreement with the results from numerical calculations.

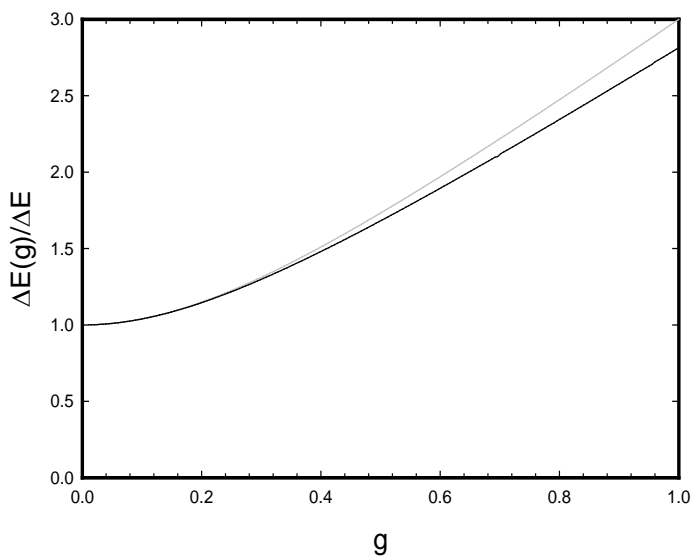


Figure 1 – Plot of  $\Delta E(g)$  as a function of  $g$  for  $\Delta E = 11\hbar\omega_0$ . Result from numerical solutions – black line; empirical result  $\sqrt{1+8g^2}$  – grey line.

### Level Anticrossing

We can study energy exchange between the two systems by focusing on the level splittings in the vicinity of an anticrossing. Consider a resonance between two states that differ by one unit of excitation in the two-level system quantum number  $m$ , and by an odd number of oscillator quanta  $n$

$$E_{n,1/2} = \frac{1}{2}\Delta E(g) + \hbar\omega_0\left(n + \frac{1}{2}\right) \quad (5)$$

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

These two states anticross when their energies are equal, which occurs when

$$\Delta E(g) = \Delta n\hbar\omega_0 \quad (6)$$

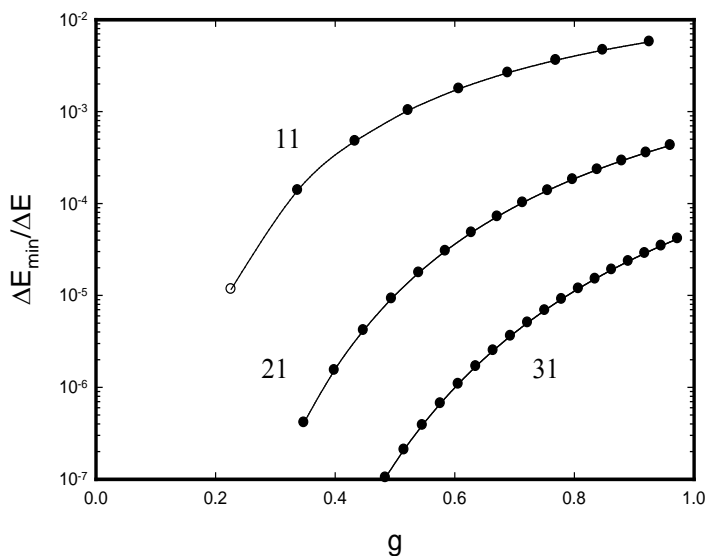


Figure 2 – Level splitting at the level anticrossing as a function of the dimensionless coupling constant  $g$ . Calculations are presented for  $\Delta E = 11\hbar\omega_0$ ,  $21\hbar\omega_0$ , and  $31\hbar\omega_0$ .

In Figure 2 we illustrate the energy splitting that occurs at the level anticrossings as a function of the dimensionless coupling strength for calculations with  $\Delta E / \hbar\omega_0 = 11, 21$ , and  $31$ . In the case of  $\Delta E = 11\hbar\omega_0$  (the top curve in Figure 2) that resonances occur for  $\Delta n$  values of 13, 15, which are indicated by the solid circles on the curve starting from the left. For example, a resonance for the conversion of one unit of two-level system excitation for 13 oscillator quanta occurs near  $g=0.22$ , with an associated level splitting of about  $10^{-5} \Delta E$ .

### Dynamics

In the vicinity of the anticrossing, the eigenfunctions are composed primarily of a mixture of the two states which anticross. On resonance, the mixing involves a 50-50 admixture of the two states, in which case the probability oscillates sinusoidally between the two states at a frequency related

to the level splitting at the anticrossing. For example, if we initialize the system in state  $\phi_{n,1/2}$ , then the subsequent occupation probabilities evolve according to

$$\begin{aligned} p_{n,1/2}(t) &= \cos^2\left(\frac{\Delta E_{\min} t}{2\hbar}\right) \\ p_{n+\Delta n,-1/2}(t) &= \sin^2\left(\frac{\Delta E_{\min} t}{2\hbar}\right) \end{aligned} \quad (7)$$

In these oscillations, the system is exchanging energy between the two-level system, which has a large transition energy, and the oscillator, which has a small characteristic energy. In the results shown in Figure 2, the rightmost point on the  $\Delta E = 31\hbar\omega_0$  curve is associated with an exchange of 85 oscillator quanta for a single dressed two-level system quantum.

## Discussion

This simple model illustrates that the simplest possible model of a single two-level system coupled to an oscillator exhibits an anomalous energy exchange effect, and that this can be demonstrated simply through a direct calculation. In order to see this effect in the spin-boson model, the dimensionless coupling constant  $g$  needs to be at least of intermediate strength. The models and solutions discussed here involved only a single two-level system coupled to an oscillator. Very similar results are obtained for a set of matched two-level systems, as long as  $n$  is large.

## Rotation

It is possible to perform a rotation of the initial Hamiltonian that produces a dressed version of the problem in which the anomalous energy exchange effect can be studied more cleanly. We can rotate to eliminate the interaction term to first order to obtain [10]

$$\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger = \hat{H}_0 + \hat{V} + \hat{W} \quad (8)$$

Here,  $\hat{H}'$  is the rotated Hamiltonian,  $\hat{U}$  is a unitary operator, and the three operators on the right are terms that we interpret as an unperturbed part of the Hamiltonian ( $\hat{H}_0$ ), and two perturbations. The unitary operator that accomplishes this rotation is



$$\hat{U} = \exp \left\{ i \arctan \left[ \frac{2V(\hat{a}^\dagger + \hat{a})}{\Delta E} \right] \frac{\hat{s}_y}{\hbar} \right\} \quad (9)$$

The unperturbed part of the rotated Hamiltonian can be written as

$$H_0 = \sqrt{\Delta E^2 + 8V^2 y^2} \frac{\hat{s}_z}{\hbar} + \hbar \omega_0 \left[ -\frac{d^2}{dy^2} + y^2 \right] \quad (10)$$

In writing this, we have used

$$y = \frac{\hat{a}^\dagger + \hat{a}}{\sqrt{2}} \quad (11)$$

The perturbation  $\hat{V}$  is given by

$$\hat{V} = i \frac{\hbar \omega_0 \sqrt{2} V}{2 \Delta E} \left\{ \frac{1}{1 + 8V^2 y^2 / \Delta E^2} \frac{d}{dy} + \frac{d}{dy} \frac{1}{1 + 8V^2 y^2 / \Delta E^2} \right\} \frac{2\hat{s}_y}{\hbar} \quad (12)$$

We may write for  $\hat{W}$

$$\hat{W} = \hbar \omega_0 \frac{V^2}{\Delta E^2} \frac{1}{[1 + 8V^2 y^2 / \Delta E^2]^2} \left( \frac{2\hat{s}_y}{\hbar} \right)^2 \quad (13)$$

### Energy levels

The rotation is useful for a number of reasons. For example, we can solve the rotated  $\hat{H}_0$  problem numerically with the result that the energy levels are given approximately by the parameterization of equation (2). In the event that the number of oscillator quanta is very large, then one can adopt a simple approximation for the eigenfunctions using SHO wavefunctions of the form

$$\phi_{n,m} = |n\rangle |s, m\rangle \quad (14)$$

This is an approximation since the exact eigenfunctions of  $\hat{H}_0$  have a spread in  $n$ . A variational estimate for the energy eigenvalues can be obtained using

$$E_{n,m} = \langle \phi_{n,m} | H_0 | \phi_{n,m} \rangle = \langle n | \sqrt{\Delta E^2 + 8V^2 y^2} | n \rangle m + \hbar \omega_0 \left( n + \frac{1}{2} \right) \quad (15)$$

This is consistent with

$$\Delta E(g) = \Delta E \langle n | \sqrt{1 + 8g^2 y^2 / n} | n \rangle \quad (16)$$

which represents an improvement over our empirical dressed energy formula above. This result is sufficiently accurate that one could not distinguish it from the numerically exact result of Figure 1 if it were added to the plot. This result is consistent with the series expansion in the large  $n$  limit reported in [15], and with the expansion reported in [17]. We have recently discussed this in [18].

### Anomalous energy exchange in the rotated problem

The energy levels of the rotated  $\hat{H}_0$  problem do not anticross, which is interesting because whatever is causing the level splitting at the anticrossing must be contained in the perturbations. We can develop a two state approximation in the rotated frame to describe the level splitting (and hence the associated dynamics). The associated eigenvalue problem can be written as

$$E \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} \frac{\Delta E(g)}{2} + \hbar \omega_0 \left( n + \frac{1}{2} \right) & \langle \phi_{n,1/2} | \hat{V} | \phi_{n+\Delta n, -1/2} \rangle \\ \langle \phi_{n+\Delta n, -1/2} | \hat{V} | \phi_{n,1/2} \rangle & -\frac{\Delta E(g)}{2} + \hbar \omega_0 \left( n + \Delta n + \frac{1}{2} \right) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \quad (17)$$

The level splitting on resonance is given by

$$\Delta E_{\min} = 2 \left| \langle \phi_{n,1/2} | \hat{V} | \phi_{n+\Delta n, -1/2} \rangle \right| \quad (18)$$

Results from this approximation are illustrated in Figure 3. One sees that the  $\hat{V}$  perturbation combined with a simple two state model leads to good agreement with numerical solutions of the initial Hamiltonian. We can understand anomalous energy exchange in this problem simply as arising from first-order transitions in the rotated frame (as discussed in [19]).

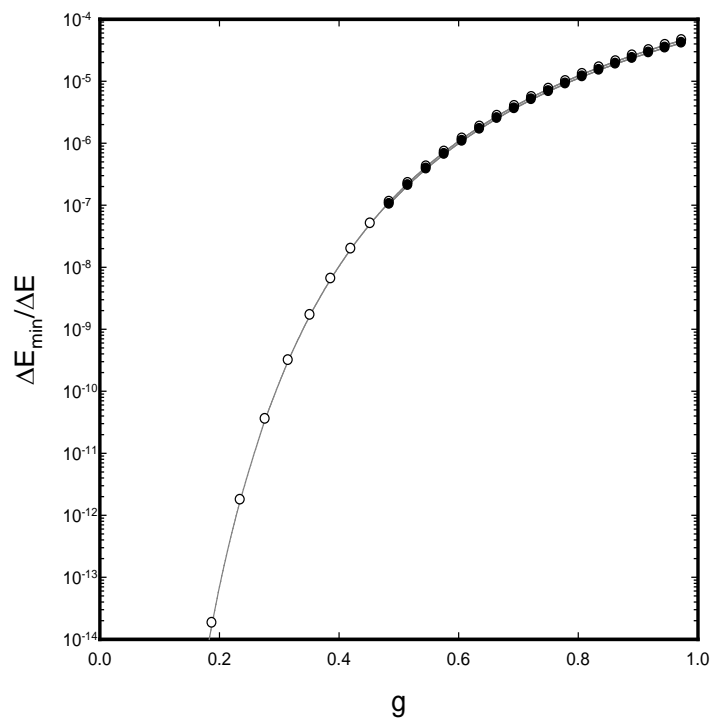


Figure 3 – Level splittings computed from a direct numerical solution of some of the resonances from the original  $\hat{H}$  problem – solid circles, and from a WKB approximation in the rotated  $\hat{H}_0$  problem to the matrix element – open circles. The parameters used in this calculation were  $\Delta E = 31\hbar\omega_0$  and  $n = 10^8$ .

### Discussion

We have found the rotated frame to be quite useful in understanding the systematics of the energy levels of the full problem, as presented here, and also in more extensive results that we do not have room to discuss. In addition, the level splittings can be understood simply in terms of matrix elements of one of the perturbations in the rotated version of the problem. The other perturbation gives a small energy shift that is not of interest in our discussion here.

## Excitation Transfer

We can use a similar model to explore excitation transfer. In this case, we couple a pair of two-level systems to an oscillator, which is accomplished using the Hamiltonian

$$\begin{aligned} \hat{H} = & \Delta E_1 \frac{\hat{s}_z^{(1)}}{\hbar} + \Delta E_2 \frac{\hat{s}_z^{(2)}}{\hbar} + \hbar\omega_0 \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \\ & + V_1 (\hat{a}^\dagger + \hat{a}) \frac{2\hat{s}_x^{(1)}}{\hbar} + V_2 (\hat{a}^\dagger + \hat{a}) \frac{2\hat{s}_x^{(2)}}{\hbar} \end{aligned} \quad (19)$$

The energy levels in this case can be approximated by

$$E_{n,m_1,m_2} = \Delta E_1(g_1)m_1 + \Delta E_2(g_2)m_2 + \hbar\omega_0 \left( n + \frac{1}{2} \right) \quad (20)$$

Where  $\Delta E_1(g_1)$  and  $\Delta E_2(g_2)$  are dressed excitation energies increased just as before. Here, there are two dimensionless coupling constants  $g_1$  and  $g_2$

$$g_1 = \frac{V_1\sqrt{n}}{\Delta E_1} \quad g_2 = \frac{V_2\sqrt{n}}{\Delta E_2} \quad (21)$$

Excitation transfer can occur in this model when the dressed excitation energy of one two-level system matches the dressed excitation energy of the other, to within an even number of oscillator quanta

$$\Delta E_2(g_2) - \Delta E_1(g_1) = \Delta n \hbar \omega_0 \quad (22)$$

In Figure 4 we show level splittings associated with excitation transfer in the case where  $\Delta E_1 = 53\hbar\omega_0$  and  $\Delta E_2 = 51\hbar\omega_0$ , with  $\Delta n = -2$ . In this calculation, we scan  $g_1$ , and search to find a  $g_2$  which gives a resonance. At the level anticrossing the two states mix, and can be described approximately using a two-state approximate as we did above. If the system is initialized at  $t=0$  in a state  $\phi_{n-1/2,1/2}$ , then the system evolves according to

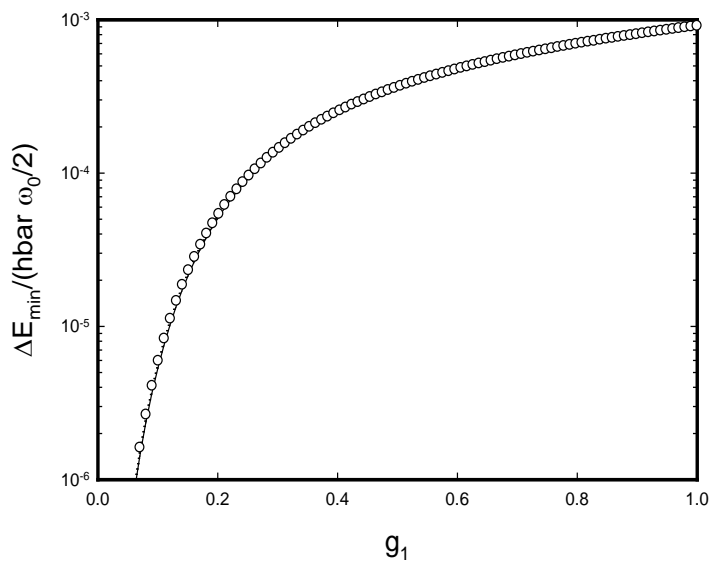


Figure 4 – Level splittings at the anticrossings for excitation transfer for  $\Delta E_1 = 53\hbar\omega_0$  and  $\Delta E_2 = 51\hbar\omega_0$  with  $\Delta n = -2$  and  $n = 10^3$ . Results are presented for direct calculations with  $\hat{H}$  as given by Equation (19) – open circles; and using perturbation theory from rotated frame solutions – solid line.

$$p_{n,-1/2,1/2}(t) = \cos^2\left(\frac{\Delta E_{\min} t}{2\hbar}\right) \quad p_{n+\Delta n,1/2,-1/2}(t) = \sin^2\left(\frac{\Delta E_{\min} t}{2\hbar}\right) \quad (23)$$

These solutions illustrate the associated coherent dynamics, and oscillation frequency is determined by the level splittings.

### Rotation

We can rotate to eliminate the coupling terms to first order as before, leading to a rotated Hamiltonian of the form [10]

$$\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger = \hat{H}_0 + \hat{V} + \hat{W} + \hat{V}_{12} \quad (24)$$

Here, the unperturbed rotated Hamiltonian  $\hat{H}_0$  is given by

$$H_0 = \sqrt{\Delta E_1^2 + 8V_1^2 y^2} \frac{\hat{s}_z^{(1)}}{\hbar} + \sqrt{\Delta E_2^2 + 8V_2^2 y^2} \frac{\hat{s}_z^{(2)}}{\hbar} + \hbar\omega_0 \left[ -\frac{d^2}{dy^2} + y^2 \right] \quad (25)$$

The perturbations  $\hat{V}$  and  $\hat{W}$  are simple generalizations of the ones we encountered previously. More interesting is the perturbation  $\hat{V}_{12}$  that mediates excitation transfer processes, for which we may write

$$\hat{V}_{12} = 2\hbar\omega_0 \frac{V_1}{\Delta E_1} \frac{V_2}{\Delta E_2} \frac{1}{(1 + 8V_1^2 y^2 / \Delta E_1^2)(1 + 8V_2^2 y^2 / \Delta E_2^2)} \frac{2s_y^{(1)}}{\hbar} \frac{2s_y^{(2)}}{\hbar} \quad (26)$$

The level splittings in this case can be approximated using the eigenfunctions of the unperturbed rotated Hamiltonian  $\hat{H}_0$  according to

$$\Delta E_{\min} = 2 \left| \langle \phi_{n,-1/2,1/2} | \hat{V}_{12} | \phi_{n+\Delta n,1/2,-1/2} \rangle \right| \quad (27)$$

One can see good agreement between this expression and level splittings computed from the original problem in the results presented in Figure 4. We have found similar agreement as long as the anticrossings are not disrupted by energy exchange resonances, which is where a two-state approximation would no longer be valid.

## Excitation Transfer and Energy Exchange

Models relevant to excess heat production in the Fleischmann-Pons experiment must implement both excitation transfer and anomalous energy exchange. We can develop very simple models that accomplish this to some degree by taking advantage of the simple Hamiltonian for a pair of two-level systems given above. In this case, we first isolate an energy exchange resonance for the second two-level system (through appropriate choices of  $\Delta E_2$  and  $g_2$ ), and then select parameters for the first two-level system for which an excitation transfer resonance exists, but for which anomalous energy exchange is weak. In general, the coupling strength for one process will not match the coupling strength for the other. In most cases, they can be matched by varying the oscillator excitation  $n$ , since the anomalous energy exchange coupling remains approximately constant in  $n$  while the excitation transfer coupling varies approximately as inverse  $n$ . We

are motivated to match the coupling strength so that we will be able to solve for the dynamics, and so that we will be able to see both effects present clearly in the solution.

Let us consider a specific example. Suppose that we first (arbitrarily) select  $\Delta E_2 = 41\hbar\omega_0$ , with  $g_2 = 0.430287$  at which an energy exchange resonance occurs (in the rotated problem) in which  $\Delta E_2(g_2) = 63\hbar\omega_0$  with a level splitting of  $1.78 \times 10^{-10} \hbar\omega_0/2$ . We then (also arbitrarily) select  $\Delta E_1 = 45\hbar\omega_0$  and  $g_1 = 0.308606$ , which causes the first two-level system to match the second with the exchange of four oscillator quanta:  $\Delta E_1(g_1) = 67\hbar\omega_0$ . It is possible to match the excitation transfer level splitting to the energy exchange level splitting (in a rotated frame calculation) using  $n = 7.72 \times 10^6$ ; which will allow us to construct an easily solvable dynamics problem as mentioned above. Energy exchange does not occur significantly with the first two-level system in this case, since with these parameters the energy splitting associated with energy exchange is lower by a factor of 6700 than the energy splitting associated with excitation transfer.

Under such conditions that the excitation transfer coupling is matched to the energy exchange coupling, with resonances occurring for both processes independently, then we can develop analytic dynamical solutions

$$\begin{aligned}
 p_{n-4,1/2,-1/2}(t) &= \left[ \frac{1 + \cos(\Delta E_{\min} t / 2\hbar)}{2} \right]^2 \\
 p_{n,-1/2,1/2}(t) &= \left[ \frac{\sin(\Delta E_{\min} t / 2\hbar)}{\sqrt{2}} \right]^2 \\
 p_{n+63,-1/2,-1/2}(t) &= \left[ \frac{1 - \cos(\Delta E_{\min} t / 2\hbar)}{2} \right]^2
 \end{aligned} \tag{28}$$

These dynamics are illustrated in Figure 5. In this example, we start with only the first two-level system excited (all states in this discussion are in the rotated frame). The system then transfers excitation (and four oscillator quanta) so that only the second two-level system is excited. Finally, the excitation of the second two-level system is transferred to the oscillator, so that neither two-level system is excited. The dynamics is coherent in this example, so that the system then proceeds to cycle back, and then repeat.

## Discussion

The importance of this model is that it illustrates clearly within the context of a slightly generalized spin-boson model (now with a pair of two-level systems) that the basic dynamics needed for describing a new physical process is present. We have excitation transfer; we have anomalous energy exchange; and the resulting dynamics is coherent.

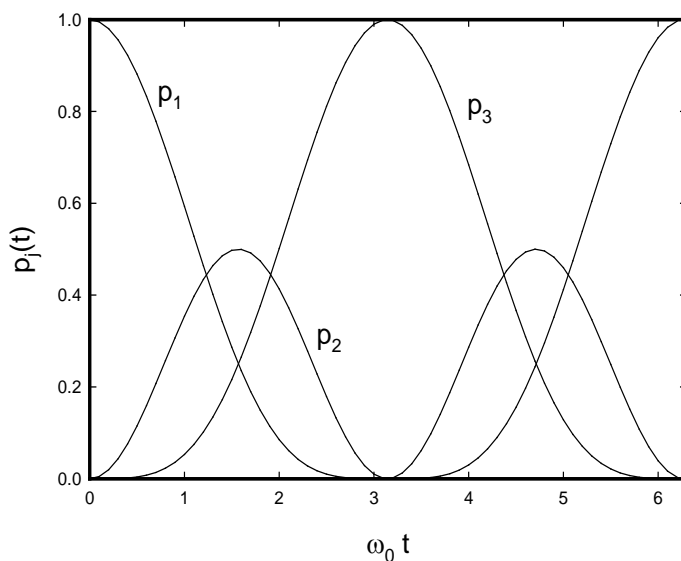


Figure 5 – Probabilities for excitation transfer followed by energy exchange under conditions where all states are degenerate in the absence of coupling, and when the coupling strengths are matched. In the first state (with probability  $p_1$ ), only the first two-level system is excited; in the second, only the second two-level system is excited; and in the third, neither two-level system is excited. The frequency  $\omega_0$  in this case is  $\Delta E_{\min} / 2\hbar$ .

## Models Augmented with Loss

The nice feature of the spin-boson type models presented above is that the system is sufficiently simple that we can isolate the excitation transfer mechanism, the energy exchange mechanism, and develop idealized models



illustrating the dynamics alone or in combination. It is also possible to extend these models to include collections of two-level systems in order to understand how the added coherence impacts the system.

However, these models seem to fall short of what is needed to account for excess heat production in the Fleischmann-Pons experiment, primarily since the associated rates are very small under conditions where  $\Delta E / \hbar\omega_0$  is greater than  $10^6$ . In essence, even though these models exhibit excitation transfer and energy exchange mechanisms, the effects are too weak in these models to do what is needed to be relevant to the excess heat problem. Something is missing.

### Excitation transfer using perturbation theory

Consider first the situation in the case of excitation transfer. We can develop an approximate analytic expression for the energy splitting using perturbation theory. We consider a finite basis approximation with six basis states corresponding to

$$\begin{aligned}\phi_1 &= |n\rangle|s,1/2\rangle|s,-1/2\rangle & \phi_2 &= |n-1\rangle|s,-1/2\rangle|s,-1/2\rangle \\ \phi_3 &= |n+1\rangle|s,-1/2\rangle|s,-1/2\rangle & \phi_4 &= |n-1\rangle|s,1/2\rangle|s,1/2\rangle \\ \phi_5 &= |n+1\rangle|s,1/2\rangle|s,1/2\rangle & \phi_6 &= |n\rangle|s,-1/2\rangle|s,1/2\rangle\end{aligned}\quad (29)$$

We assume that  $\phi_1$  and  $\phi_6$  are resonant in the absence of coupling [ $\Delta E_1(g_1) = \Delta E_2(g_2)$ ]. The finite basis equations for the expansion coefficients  $c_1 \dots c_6$  can be written as

$$\begin{aligned}Ec_1 &= H_1c_1 + V_1\sqrt{nc_2} + V_1\sqrt{n+1}c_3 + V_2\sqrt{nc_4} + V_2c_5 \\ Ec_2 &= H_2c_2 + V_1\sqrt{nc_1} + V_2\sqrt{nc_6} \\ Ec_3 &= H_3c_3 + V_1\sqrt{n+1}c_1 + V_2\sqrt{n+1}c_6 \\ Ec_4 &= H_4c_4 + V_2\sqrt{nc_1} + V_1\sqrt{nc_6} \\ Ec_5 &= H_5c_5 + V_2\sqrt{n+1}c_1 + V_1\sqrt{n+1}c_6 \\ Ec_6 &= H_6c_6 + V_2\sqrt{nc_2} + V_2\sqrt{n+1}c_3 + V_1\sqrt{nc_4} + V_1\sqrt{n+1}c_5\end{aligned}\quad (30)$$

We can eliminate the interior states  $\phi_2$  through  $\phi_5$  to obtain a reduced set of equations of the form

$$\begin{aligned}
Ec_1 &= H_1c_1 + \Sigma_1(E)c_1 + V_{16}(E)c_6 \\
Ec_6 &= H_6c_6 + \Sigma_6(E)c_6 + V_{61}(E)c_1
\end{aligned} \tag{31}$$

The level splitting under resonant conditions in this model is

$$\Delta E_{\min} = 2\sqrt{|V_{16}(E)V_{61}(E)|} \tag{32}$$

An explicit calculation produces the result in this case that

$$\begin{aligned}
V_{16}(E) &= V_{61}(E) = V_1V_2 \left[ \frac{n}{E-H_2} + \frac{n+1}{E-H_3} + \frac{n}{E-H_4} + \frac{n+1}{E-H_5} \right] \\
&\approx \frac{2\hbar\omega_0V_1V_2}{(\Delta E_1)^2 - (\hbar\omega_0)^2}
\end{aligned} \tag{33}$$

This approximation gives good results for the level splitting associated with excitation transfer in the limit of small  $g_1$  and  $g_2$ .

### Inclusion of loss effects into the model

In the intermediate states  $\phi_2$  and  $\phi_3$  above, both of the two-level systems are unexcited; hence, the coupled quantum system has available an energy  $E$  which is much greater than either of the basis state energies  $H_2$  and  $H_3$ . In this case, if there exist loss channels for the oscillator at decay energies near the dressed two-level system energies, one would expect the system to undergo incoherent decay to these states. The existence of such decay modes has a dramatic impact on the model, which we need to include.

To do so, we augment the Hamiltonian to include loss

$$\begin{aligned}
\hat{H} &= \Delta E_1 \frac{\hat{s}_z^{(1)}}{\hbar} + \Delta E_2 \frac{\hat{s}_z^{(2)}}{\hbar} + \hbar\omega_0 \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) - \frac{i\hbar}{2} \hat{\Gamma}(E) \\
&\quad + V_1 (\hat{a}^\dagger + \hat{a}) \frac{2\hat{s}_x^{(1)}}{\hbar} + V_2 (\hat{a}^\dagger + \hat{a}) \frac{2\hat{s}_x^{(2)}}{\hbar}
\end{aligned} \tag{34}$$

Here, the spin-boson model that we have been considering has been augmented with a loss term that implements the effect under discussion. For a more

complete discussion of loss mechanisms and the development of relevant loss models, see Hagelstein and Chaudhary [10].

### Enhancement of excitation transfer

With the inclusion of loss terms in the model, the model undergoes qualitative changes. We can see this in the modification of the perturbation theory for excitation transfer discussed above. Let us now include loss for states  $\phi_2$  and  $\phi_3$ , which we can do in a simple way by using a constant loss model. We write for these basis states

$$\begin{aligned} Ec_2 &= \left( H_2 - \frac{i\hbar\Gamma}{2} \right) c_2 + V_1 \sqrt{n} c_1 + V_2 \sqrt{n} c_6 \\ Ec_3 &= \left( H_3 - \frac{i\hbar\Gamma}{2} \right) c_3 + V_1 \sqrt{n+1} c_1 + V_2 \sqrt{n+1} c_6 \end{aligned} \quad (35)$$

When these states are eliminated, we still recover a reduced two-state model; however, the indirect coupling coefficients are now changed. We may write

$$V_{16}(E) = V_1 V_2 \left[ \frac{n}{E - H_2 + i\hbar\Gamma/2} + \frac{n+1}{E - H_3 + i\hbar\Gamma/2} + \frac{n}{E - H_4} + \frac{n+1}{E - H_5} \right]$$

In the event that the loss term becomes very large ( $\Gamma \rightarrow \infty$ ), then

$$V_{16}(E) \approx -\frac{2V_1 V_2 \Delta E_1 (g_1) n}{(\Delta E_1)^2 - (\hbar\omega_0)^2} \quad (36)$$

This is orders of magnitude larger than what we found above in the lossless version of the model. We see that the inclusion of loss breaks the destructive interference that was initially present, and that is the reason.

## Discussion and Conclusions

Our discussion has focused primarily on simple spin-boson type models that illustrate excitation transfer and anomalous energy exchange effects. These

effects are of interest to us in general since they are required in the development of models for excess heat in the Fleischmann-Pons experiment.

We require the excitation transfer mechanism in order to violate local energy conservation (but retain global energy conservation) in the initial step of the reaction. Two deuterons interact to make  $^4\text{He}$ , exchanging one or more phonons in the process, with the reaction energy transferred elsewhere. The coupling in this case is weak, since the transition is hindered by the presence of a Gamow factor due to coupling through the Coulomb barrier.

We require the anomalous energy exchange mechanism since there are no energetic particles observed commensurate with the energy produced. This energy exchange mechanism works through the exchange of a single oscillator quantum in association with every interaction (excitation transfer steps, or self-interaction steps, within the second set of equivalent two-level systems). It accomplishes the exchange of a large energy quantum associated with the two-level systems into a large number of low energy quanta associated with the oscillator. Both the excitation transfer effect and the anomalous energy exchange effect involve coherent dynamics within the models presented here, and within a larger set of models that we have investigated so far.

The lossless models are of interest as we have mentioned previously since we are able to set up simple models that exhibit each effect individually or both together. We are able to isolate the specific perturbation in the rotated Hamiltonian that mediates excitation transfer, and also the specific perturbation that mediates anomalous energy exchange. The effects can be studied in terms of direct solutions of the initial spin-boson type of Hamiltonian  $\hat{H}$ ; from numerical and approximate solutions of the rotated unperturbed Hamiltonian  $\hat{H}_0$ ; using the WKB approximation on the rotated problem; and through other methods as well. For example, in the text we discussed briefly an example in which we are able to develop an analytic solution for a problem in which excitation transfer is followed coherently by anomalous energy exchange where a total of 67 oscillator quanta make up the dressed transition energy of the first two-level system.

The lossless version of the problem results in simple toy models that we can analyze as we please, although it is probably clear from the specific examples that we considered that these models fall short of what is needed for modeling excess heat production. These toy problems also require very precise resonances to be present for any of the effects to occur, which seems not to be consistent qualitatively with excess heat observations.

Augmenting the models with loss changes things dramatically, as we have discussed briefly in the case of excitation transfer. The rate at which excitation transfer occurs in the lossy models is greatly enhanced, and also the rate at which anomalous energy exchange occurs is similarly enhanced. Lossy models can show both effects readily, even without resonant conditions being satisfied.

To connect these models to excess heat production experiments (in PdD), we identify a molecular D<sub>2</sub> state in the vicinity of a host atom vacancy as the upper state of the first two-level system(s), and <sup>4</sup>He with the lower state. The lower state of the second two-level system(s) we identify with ground state nuclei present in the host. Experiment so far does not make clear what excited nuclear states should be identified with the upper state of the second two-level system(s). Theoretical arguments point to excited states composed of a neutral particle and daughter; for example, a neutron plus <sup>3</sup>He in the case of a <sup>4</sup>He ground state; or <sup>106</sup>Pd plus a tetra-neutron in the case of a <sup>110</sup>Pd ground state. Such excited states are favored due to the ability of the lattice to exchange phonons in transitions from the ground state. However, it remains to establish that such states can be stabilized sufficiently for the schemes under discussion to work properly.

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