



Research Article

# Dynamics in the Case of Coupled Degenerate States

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## Abstract

Excess heat in the Fleischmann–Pons experiment has been observed in a great many experiments, and we have been working toward the development of a theoretical model to account for it. In the experiments, excess heat is correlated with  $^4\text{He}$ , but there are no commensurate energetic particles. This has motivated us to consider models in which the excess energy is communicated directly to low energy degrees of freedom associated with the solid state environment. We have found relatively simple models which are capable of splitting up a large energy quantum into a very large number of much smaller energy quanta. In order to analyze these new models, we are motivated to consider the dynamics associated with a set of ordered degenerate states with nearest neighbor coupling.

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*Keywords:* Coherent dynamics, Degenerate states, Excess heat, Fleischmann–Pons experiment, Lossy spin-boson model

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## 1. Introduction

There has been a keen interest in the elucidation of the underlying mechanism associated with excess heat in the Fleischmann–Pons experiment [1,2] over the past two decades, and there have been a great many papers put forth over the years suggesting how it might work. Some years ago Takahashi and coworkers gave a simple overview of the situation, wherein was described four scenarios [3]. These included aneutronic fusion with hidden reaction products, fusion with the energy coupled directly to the lattice, chemical or mechanical explanations, or experimental error. Enough experimental confirmations of the effect have been reported that it seems unlikely that we are dealing with experimental error [4,5]. The amount of energy observed is sufficiently large that chemical or mechanical explanations seem impossible, and there is no indication of chemical reaction products or mechanical changes commensurate with the energy produced. Recently we were able to make strong arguments against the possibility of hidden energetic products from proposed aneutronic fusion reactions, since they would produce secondary neutrons in sufficient quantities to have

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been readily observed [6]. Among Takahashi's scenarios, the one that remains (coupling the nuclear energy directly to the lattice) has been the focus of our efforts for many years now.

Of course, the theorists have been busy since publication of the different scenarios by Takahashi et al (for example, see [5,7]), and it is likely that at present a revised list of scenarios is appropriate. From our perspective, the constraints imposed from the upper limits of energetic reaction products [6] are sufficiently severe that the majority of mechanisms that have been proposed since 1989 can be ruled out as inconsistent with experiment. At this point there seem to be two kinds of candidates that remain. One of these are schemes which involve direct coupling of energy to the lattice, or to other condensed matter degrees of freedom (such as plasmon modes [8], or hybrid plasmon–phonon modes). The other are schemes in which an extreme fractionation of the nuclear energy occurs into kinetic energy of a very large number of nuclei, as argued for by Kim [9]. Our concern with this approach is that a mechanism through which this might occur has not yet been clarified.

We have been interested for some time in the problem of how a large quantum can be split up into a very large number of small quanta. To study this problem, we first focused on the spin-boson model [10–12] and variants. In the spin-boson model, two-level systems and an oscillator are coupled, with an interaction that is linear in the sense that one transition of the two-level systems occurs with the exchange of a single oscillator quantum. It has been understood for many years that this model described coherent energy exchange in the multiphoton regime, in which many oscillator quanta are exchanged for a single two-level system quantum [13,14]. The transition rates in this model are slow because of destructive interference effects. We found that the destructive interference could be removed in part if loss terms are included, resulting in an enhancement by many orders of magnitude of the associated rate for coherent energy exchange [15].

In this work we are interested in the dynamics of coherent energy exchange in this and related models. We might think of coherent energy exchange in the limit where many oscillator quanta are exchanged as occurring as a result of nearly degenerate states which are weakly coupled through off-resonant transitions through intermediate states. We would expect the resulting system dynamics when the indirect coupling is strong to be similar to that of a chain of degenerate states with nearest neighbor coupling. This leads to a quantum mechanical problem that we can analyze relatively simply. In the event that there is a small systematic mismatch between the nearly degenerate levels, we are also able to recover useful evolution equations.

We note that the first reviewer for this paper had numerous criticisms. With encouragement from colleagues, we have included selected criticisms with responses in Appendix C.

## 2. A Basic Model for Coupling between Degenerate States

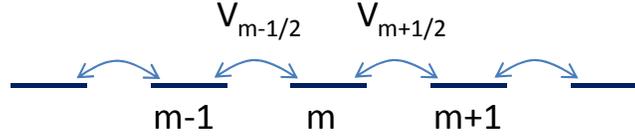
We begin by considering a highly idealized model for a quantum system that evolves through coupling between ordered degenerate states. We assume that the dynamics are governed by a Hamiltonian  $\hat{H}$  so that

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi, \quad (1)$$

We assume the wavefunction  $\Psi$  can be expanded in terms of a set of degenerate basis states

$$\Psi = \sum_m c_m(t) |\Phi_m\rangle. \quad (2)$$

We assume that the dynamics of the system can be reasonably approximated by coupling only between nearest neighbors (see Fig. 1), so that



**Figure 1.** Schematic of ordered degenerate states with nearest neighbor coupling.

$$i\hbar \frac{d}{dt} c_m(t) = V_{m+\frac{1}{2}} c_{m+1}(t) + V_{m-\frac{1}{2}} c_{m-1}(t). \quad (3)$$

This presumes that the energies are degenerate

$$\langle \Phi_m | \hat{H} | \Phi_m \rangle = 0, \quad (4)$$

where we have removed any finite offset from our model Hamiltonian for simplicity. The coupling coefficients  $V_{m\pm\frac{1}{2}}$  are the matrix elements

$$V_{m\pm\frac{1}{2}} = \langle \Phi_m | \hat{H} | \Phi_{m\pm 1} \rangle, \quad (5)$$

which we take to be real in our model.

Equation (3) defines the basic model of interest to us here. One might argue that the assumptions of the model are restrictive, so that there are only a few quantum systems that work this way. However, it may be the case that the simplified model under discussion here is one that has been extracted from a much more complicated model, that the focus is on a small subset of the states which are degenerate, and the effect of all the other states has been included through indirect coupling in the model Hamiltonian  $\hat{H}$ . This will be our point of view, although it will not be required in the discussion which follows in this work.

In the particular case of two-level systems coupled to an oscillator (a case that we will analyze later on in this paper), the degenerate states are those in which energy is kept constant by maintaining constant  $m\Delta E + n\hbar\omega_0$ , where  $\Delta E$  is the two-level system transition energy and where  $\hbar\omega_0$  is the characteristic energy of the oscillator. In this case, the degenerate states are indirectly coupled since many oscillator quanta need to be exchanged in order to make up for the change of a single two-level system.

### 3. Evolution Equation for $\langle m \rangle$

Let us define the average  $\langle m \rangle$  according to

$$\langle m \rangle = \sum_m m |c_m|^2. \quad (6)$$

To understand the dynamics of the system, we would like to know how  $\langle m \rangle$  changes with time. As a result, we are interested in the calculation of the derivative. As a first step we may write

$$\frac{d}{dt}\langle m \rangle = \sum_m m \left( \frac{dc_m^*}{dt} c_m + c_m^* \frac{dc_m}{dt} \right). \quad (7)$$

We evaluate to obtain

$$\begin{aligned} \frac{d}{dt}\langle m \rangle &= -\frac{1}{i\hbar} \sum_m m (V_{m-1/2} c_{m-1}^* + V_{m+1/2} c_{m+1}^*) c_m \\ &\quad + \frac{1}{i\hbar} \sum_m m c_m^* (V_{m-1/2} c_{m-1} + V_{m+1/2} c_{m+1}). \end{aligned} \quad (8)$$

We can recast this as

$$\begin{aligned} \frac{d}{dt}\langle m \rangle &= \frac{1}{i\hbar} \sum_m m (c_m^* c_{m+1} - c_{m+1}^* c_m) V_{m+\frac{1}{2}} \\ &\quad + \frac{1}{i\hbar} \sum_m m (c_m^* c_{m-1} - c_{m-1}^* c_m) V_{m-\frac{1}{2}}, \end{aligned} \quad (9)$$

which simplifies to

$$\frac{d}{dt}\langle m \rangle = -\frac{1}{i\hbar} \sum_m V_{m+1/2} (c_m^* c_{m+1} - c_{m+1}^* c_m). \quad (10)$$

It is convenient to define the average velocity  $\langle \hat{v} \rangle$  according to

$$\langle \hat{v} \rangle = -\frac{1}{i\hbar} \sum_m V_{m+1/2} (c_m^* c_{m+1} - c_{m+1}^* c_m). \quad (11)$$

This allows us to write

$$\frac{d}{dt}\langle m \rangle = \langle \hat{v} \rangle. \quad (12)$$

In general we can identify  $\langle \hat{v} \rangle$  with the rate for transitions between the different nearly degenerate states.

#### 4. Evolution Equation for $\langle \hat{v} \rangle$

Next, we require an evolution equation for the average velocity. We write

$$\frac{d}{dt}\langle \hat{v} \rangle = -\frac{1}{i\hbar} \sum_m V_{m+1/2} \left( \frac{dc_m^*}{dt} c_{m+1} + c_m^* \frac{dc_{m+1}}{dt} - \frac{dc_{m+1}^*}{dt} c_m - c_{m+1}^* \frac{dc_m}{dt} \right). \quad (13)$$

We substitute to obtain

$$\begin{aligned}
\frac{d}{dt}\langle\hat{v}\rangle &= \frac{2}{(i\hbar)^2} \sum_m V_{m+\frac{1}{2}}^2 (|c_{m+1}|^2 - |c_m|^2) \\
&+ \frac{1}{(i\hbar)^2} \sum_m V_{m+\frac{1}{2}} V_{m-\frac{1}{2}} (c_{m-1}^* c_{m+1} + c_{m+1}^* c_{m-1}) \\
&- \frac{1}{(i\hbar)^2} \sum_m V_{m+\frac{1}{2}} V_{m+\frac{3}{2}} (c_m^* c_{m+2} + c_{m+2}^* c_m).
\end{aligned} \tag{14}$$

We can collect terms and rearrange to obtain

$$\frac{d}{dt}\langle\hat{v}\rangle = -\frac{2}{(i\hbar)^2} \sum_m (V_{m+1/2}^2 - V_{m-1/2}^2) |c_m|^2. \tag{15}$$

It seems reasonable to introduce the notation

$$\left\langle \frac{dV^2}{dm} \right\rangle = \sum_m (V_{m+1/2}^2 - V_{m-1/2}^2) |c_m|^2. \tag{16}$$

The resulting evolution equation takes the form

$$\frac{d}{dt}\langle\hat{v}\rangle = \frac{2}{\hbar^2} \left\langle \frac{dV^2}{dm} \right\rangle. \tag{17}$$

Note that the velocity increases towards regions where the magnitude of the coupling constant is larger.

#### 4.1. Discussion

We are familiar with the evolution equations for the closely related problem of the dynamics of spin systems (which is discussed in Appendix A). The evolution equations that we developed in this section and in the previous section constitute an interesting and nontrivial generalization of this model.

Several interesting features of this generalization can be observed. One feature is that we have obtained only two independent evolution equations, which is significant since had we chosen a somewhat more complicated model we could have easily generated an infinite set. Another is that the resulting equations are of the general form of Newton's laws in one dimension, which allows us to apply our intuition about classical particle dynamics in one dimension to this new problem involving coupling between ordered degenerate basis states. Finally we see that the coupling matrix elements  $V_{m+1/2}$  determine the dynamics in a fundamental way. Hence when we analyze new models that involve a set of coupled degenerate basis states, our attention should properly be focused on these coupling matrix elements. With an understanding of these coupling matrix elements, we can predict the associated dynamics simply.

### 5. Analogy with Kinetic and Potential Energy

Since the evolution equations are of the same form as classical Newton's laws in one dimension, we can develop an effective energy equation for the classical version of the problem. To proceed, we identify the classical position  $m(t)$  and velocity  $v(t)$  with the average values

$$\langle m \rangle \rightarrow m(t), \quad \langle \hat{v} \rangle \rightarrow v(t). \quad (18)$$

The classical equations are

$$\begin{aligned} \frac{d}{dt}m(t) &= v(t), \\ \frac{d}{dt}v(t) &= \frac{2}{\hbar^2} \frac{dV^2}{dm}. \end{aligned} \quad (19)$$

The associated energy equation is then approximately

$$C = \frac{1}{2}v^2 - \frac{2}{\hbar^2}V^2(m). \quad (20)$$

From this it is possible to determine the velocity as a function of position as

$$v = \pm \sqrt{2C + \frac{4}{\hbar^2}V^2(m)}. \quad (21)$$

This is analogous to the situation in classical dynamics where we can specify the momentum at each position from a knowledge of the potential and total energy.

In some cases, the coupling becomes weaker for the outer values of  $m$ . If so, then for a trajectory that starts at these outer values it should be a reasonable approximation that  $C$  is small (since the velocity is small where the coupling is very weak). For zero  $C$  we obtain

$$v(m) = \pm \frac{2}{\hbar} V(m). \quad (22)$$

This formula is important since we can specify the velocity  $v$  (which is the rate for transitions between the different nearly degenerate states) directly in terms of the coupling matrix elements as a function of  $m$ . If the velocity is a sufficiently simple function of  $m$ , then we might be able to integrate to obtain an explicit expression for  $m(t)$ .

The maximum rate in this approximation occurs where the coupling matrix element is maximum, with a value of

$$\max(v) = \frac{2}{\hbar} \max |V(m)|. \quad (23)$$

## 6. Dynamics of Coherent Energy Exchange in the Perturbative Limit

In a previous work [15] we analyzed indirect coupling matrix elements for the spin-boson model augmented with loss using perturbation theory. We can make use of these results to calculate the associated system dynamics. In the event that there are a very large number of two-level systems, then it is possible to arrange for a version of the problem in which the indirectly coupled states are very nearly degenerate. In this case we can make use of the equivalent classical evolution equations from the section above

$$\frac{d^2}{dt^2}m(t) = \frac{2}{\hbar^2} \frac{d}{dm} V^2(m). \quad (24)$$

It seems reasonable to take as an example the perturbation theory model where one two-level system quantum is exchanged for five oscillator quanta. In this case we developed explicit formulas for the indirect coupling matrix elements which can be used directly to evaluate the evolution.

### 6.1. Large $S$ and $n$ approximation

The explicit expressions for the indirect coupling constants are complicated, so that the equation that results from taking the difference of the squares to determine the acceleration will be more complicated. We seek a simplification of the problem relevant to the large  $S$  limit. A common approximation is to neglect terms of order unity in the Dicke factors, so that

$$\sqrt{(S \mp m)(S \pm m + 1)} \rightarrow \sqrt{(S^2 - m^2)}. \quad (25)$$

Using this kind of approximation, we can write

$$F(S, M) \rightarrow \frac{7}{36}(S^2 - m^2)^2 \quad (26)$$

$$V_{1,12}(E) \rightarrow \frac{625}{64} \frac{(V\sqrt{n})^5}{\Delta E^4} \sqrt{(S^2 - m^2)} \quad (\Gamma = 0), \quad (27)$$

where we have assumed that  $n$  is large. The indirect coupling in the lossy limit is then approximated by

$$V_{1,12}(E) \rightarrow \frac{4375}{2304} \frac{(V\sqrt{n})^5}{\Delta E^4} (S^2 - m^2)^{\frac{5}{2}} \quad (\Gamma = \infty). \quad (28)$$

### 6.2. Approximation for the force

We can use the estimate for the indirect coupling in order to estimate the force. We may write

$$\begin{aligned} \frac{d}{dm} V^2(m) &= \left( \frac{4375}{2304} \right)^2 \frac{(V\sqrt{n})^{10}}{\Delta E^8} \frac{d}{dm} (S^2 - m^2)^5 \\ &= -10 \left( \frac{4375}{2304} \right)^2 \frac{(V\sqrt{n})^{10}}{\Delta E^8} m (S^2 - m^2)^4. \end{aligned} \quad (29)$$

The dynamics for the classical version of the problem is then described by

$$\frac{d^2}{dt^2}m(t) = -20 \left( \frac{4375}{2304} \right)^2 \frac{(V\sqrt{n})^{10}}{\hbar^2 \Delta E^8} m(t) [S^2 - m^2(t)]^4. \quad (30)$$

### 6.3. Simplification

It is convenient to recast the problem in terms of a normalized version of  $m(t)$

$$y(t) = \frac{m(t)}{S}, \quad (31)$$

which allows us to write

$$\frac{d^2}{dt^2}y(t) = -\Omega_0^2 y(t)[1 - y^2(t)]^4, \quad (32)$$

where the characteristic frequency  $\Omega_0$  is defined through

$$\Omega_0^2 = 20 \left( \frac{4375}{2304} \right)^2 \frac{(V\sqrt{n})^{10}}{\hbar^2 \Delta E^8} S^8. \quad (33)$$

### 6.4. Solutions

The nonlinear second-order classical equation (Eq. (32)) has oscillatory solutions (which correspond to a ball rolling back and forth confined in a nonlinear well) and a non-oscillatory solution (corresponding to a ball with an energy matched to the top of the well). The latter solution is illustrated in Fig. 2. This function can be fit well according to

$$y(t) = -\frac{ax + bx^3}{1 + bx^2\sqrt{c + x^2}} \quad (34)$$

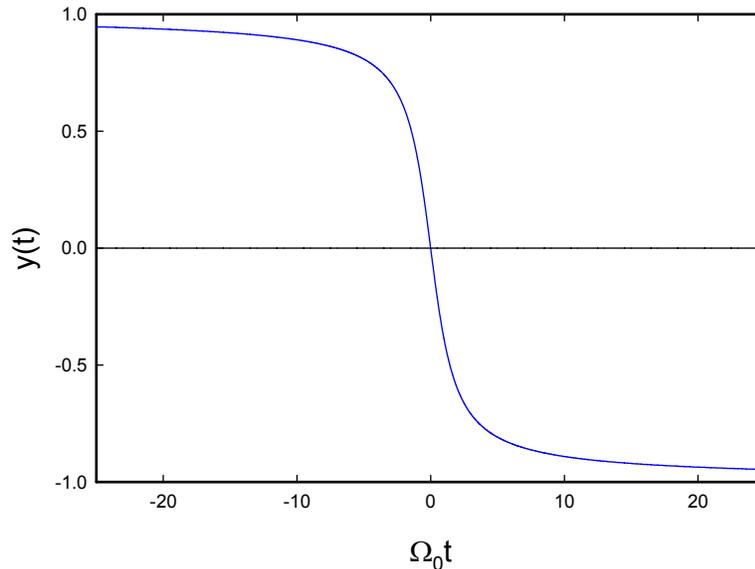
with

$$a = 0.381902, \quad b = 0.00708607, \quad c = 161.393. \quad (35)$$

## 7. Summary and Conclusions

We are interested in developing models for excess heat in the Fleischmann–Pons experiment, as outlined in the Introduction. The key problem from our perspective in the development of relevant models is that of coherent energy exchange under conditions where a large energy quantum is split up into a very large number of smaller energy quanta. We have proposed models that accomplish this, and which begin to be relevant to the new effect. However, these new models are not so easy to analyze in general. To make progress on them, we have found that some understanding is possible by considering a subset of the states which are nearly degenerate, and then developing models which account for the indirect coupling between these nearly degenerate states. Once this is done, then we are able to understand what the new models do, and we are able to extract estimates for the reaction rates from them. From this point of view, it seems that the place to start in our discussion of the new models is by examining the dynamics associated with a set of ordered degenerate states with nearest neighbor coupling. This is the simple model we have introduced in Section 2.

We find that the resulting evolution equations for this model are simple, and are of the form of Newton's laws in one dimension. We find that the dynamics are determined ultimately by the coupling matrix elements between the different nearly degenerate basis states, hence in studying such models our attention will naturally be drawn to these coupling



**Figure 2.** Schematic of ordered states with constant energy separation, and with nearest neighbor coupling..

matrix elements. We have tested them against a well-known problem involving spin dynamics in Appendix A, and we have verified that we get the right answer. Since the evolution equations are similar to Newton's laws, we can construct an energy expression for the equivalent classical problem. This allows us to specify the velocity, or coherent reaction rate, as a function of the index given an equivalent energy. Explicit results were given for the dynamics of a spin-boson model augmented with loss, where we made use of the indirect coupling matrix elements calculated in an earlier work. This provides an example which shows how the approach under discussion can be used to describe the dynamics of coherent energy exchange in the multiphonon regime.

The requirement of precise energy degeneracy is restrictive. In general, if the states are not degenerate, then the dynamics become very complicated. However, in the special case where the basis state energies are linear in the index, it is possible to develop somewhat more general evolution equations which are similar in form to those found in the dynamics of a spin system (see Appendix B). The absence of degeneracy in this model results in the presence of a reactive term which impacts the velocity.

### Appendix A. Spin Dynamics Example

To see whether the simple model developed above works, we would like to try it out on a test problem for which the answer is known.

#### Appendix A.1. Test problem

In this case, an obvious test problem is the dynamics of a system of many equivalent spins governed by a simple Hamiltonian. For the test problem, we take the Hamiltonian to be

$$\hat{H}_T = 2\Omega\hat{S}_x. \quad (\text{A.1})$$

We can make use of the commutation relations of the spin operators to write

$$\frac{d}{dt}\langle\hat{S}_z\rangle = \frac{2\Omega}{i\hbar}\langle[\hat{S}_z, \hat{S}_x]\rangle = \Omega\langle\hat{S}_y\rangle. \quad (\text{A.2})$$

Similarly, we may write

$$\frac{d}{dt}\langle\hat{S}_y\rangle = \frac{2\Omega}{i\hbar}\langle[\hat{S}_y, \hat{S}_x]\rangle = -\Omega\langle\hat{S}_z\rangle. \quad (\text{A.3})$$

#### Appendix A.2. Dynamics from the spin operators

To make a connection with our test problem, we can identify

$$\langle m \rangle = \frac{\langle\hat{S}_z\rangle}{\hbar}, \quad \langle \hat{v} \rangle = \frac{\Omega\langle\hat{S}_y\rangle}{\hbar}. \quad (\text{A.4})$$

With these definitions we obtain the exact equations

$$\begin{aligned} \frac{d}{dt}\langle m \rangle &= \langle \hat{v} \rangle, \\ \frac{d}{dt}\langle \hat{v} \rangle &= -\Omega^2\langle m \rangle. \end{aligned} \quad (\text{A.5})$$

#### Appendix A.3. Dynamics from coupled degenerate states

To make use of the approach from above based on degenerate states, we first require evaluation of the spin matrix element

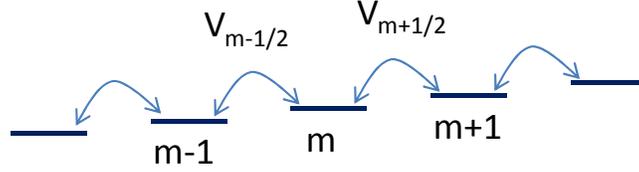
$$V_{m+\frac{1}{2}} = \langle S, m | 2\Omega\hat{S}_x | S, m+1 \rangle = \hbar\Omega\sqrt{(S-m)(S+m+1)}, \quad (\text{A.6})$$

$$V_{m-\frac{1}{2}} = \langle S, m | 2\Omega\hat{S}_x | S, m-1 \rangle = \hbar\Omega\sqrt{(S+m)(S-m+1)}. \quad (\text{A.7})$$

We can use these to compute

$$\begin{aligned} V_{m+\frac{1}{2}}^2 - V_{m-\frac{1}{2}}^2 &= (\hbar\Omega)^2 \left[ (S-m)(S+m+1) - (S+m)(S-m+1) \right] \\ &= -2(\hbar\Omega)^2 m. \end{aligned} \quad (\text{A.8})$$

The spin dynamics computed using from the dynamics above is then



**Figure 3.** Schematic of ordered states with constant energy separation, and with nearest neighbor coupling.

$$\begin{aligned}\frac{d}{dt}\langle m \rangle &= \langle \hat{v} \rangle, \\ \frac{d}{dt}\langle \hat{v} \rangle &= -\Omega^2 \langle m \rangle\end{aligned}\quad (\text{A.9})$$

in agreement with the dynamics obtained from the spin commutation relations.

### Appendix B. Generalization to a Non-degenerate Set of States

For more sophisticated models it may be that the levels are not strictly degenerate, in which case the dynamics quickly becomes much more complicated. It is possible to provide an extension of the dynamical equations for the simplest generalization to the non-degenerate case where the basis state energy increases linearly in the index (see Fig. 3). The associated model is described by

$$i\hbar \frac{d}{dt}c_m(t) = \delta E m c_m(t) + V_{m+\frac{1}{2}}c_{m+1}(t) + V_{m-\frac{1}{2}}c_{m-1}(t). \quad (\text{B.1})$$

The evolution equations now become

$$\begin{aligned}\frac{d}{dt}\langle m \rangle &= \langle \hat{v} \rangle, \\ \frac{d}{dt}\langle \hat{v} \rangle &= \frac{2}{\hbar^2} \left\langle \frac{dV^2}{dm} \right\rangle + \langle \hat{w} \rangle, \\ \frac{d}{dt}\langle \hat{w} \rangle &= -2 \left( \frac{\delta E}{\hbar} \right)^2 \langle \hat{v} \rangle.\end{aligned}\quad (\text{B.2})$$

The average value  $\langle \hat{w} \rangle$  is defined by

$$\langle \hat{w} \rangle = \frac{2\Delta E}{\hbar^2} \sum_m V_{m+\frac{1}{2}} (c_m^* c_{m+1} + c_{m+1}^* c_m). \quad (\text{B.3})$$

These equations are closely related to the evolution equations obtained for spin systems, but they can provide estimates for the dynamics for more complicated models.

## Appendix C. Responses to Reviewer Comments

The first reviewer put forth a great many criticisms of this paper and the preceding one [15]. Our colleagues provided encouragement to include some of the associated criticisms and responses in the papers. In response, we have provided a selection of the reviewer’s criticisms, modified where appropriate to be more understandable, as well as some discussion of the associated issues.

### Appendix C.1. No reason to focus on degenerate states

*There is no reason to have degenerate states, which seems merely a “desired assumption” by the authors.*

What we mean by degenerate states in the context of the lossy spin-boson model are basis states with constant energy

$$E = m\Delta E + \Delta n\hbar\omega_0.$$

For example, suppose that we start with a state with  $m$  two-level systems excited, and  $n$  oscillator quanta. To go to a degenerate state with  $m - 1$  two-level systems excited, we are going to have to have an increase in the oscillator energy by  $\Delta n$  oscillator quanta, where  $\Delta n$  is the ratio the two-level transition energy and the characteristic oscillator energy. More simply, if the two-level transition energy is matched to five oscillator quanta, then you need to increase the oscillator energy by five quanta every time you lose one excited state of the two-level systems.

Hence, the “desired” assumption in this case is that we would like to conserve energy overall between the two-level systems and the oscillator.

### Appendix C.2. No reason to focus on indirect coupling

*There is no reason to have indirect coupling, which also seems merely a “desired assumption”.*

In the spin-boson model, there is no direct coupling between these degenerate states in the multiphoton regime, which we are working in. As a result, the coupling is indirect. This is explained in the papers, and we have presented an explicit perturbation theory calculation as a concrete example. The coupling under discussion in the spin-boson model is due to phonon exchange, and we are able to derive this directly from more general Hamiltonians.

### Appendix C.3. Nuclear reactions are irreversible

*Nuclear reactions are irreversible (one-way for out-going channel with significant mass-energy defect) and are stochastic processes (namely one-way or never-return for going out to final interaction products with big entropy increase). So the assumed oscillatory dynamics between the two states (where energy is transferred from the nuclear system to the oscillator) cannot exist, due to the stochastic one-way nuclear decay.*

In the simple models discussed in this paper, the dynamics can be oscillatory in the sense that the energy can go from the two-level systems to the oscillator and back again, coherently. This is consistent generally with how coherent dynamics tend to work.

The reviewer has decided that one cannot apply models with this kind of dynamics to a nuclear transition, seemingly because conventional (incoherent) nuclear reactions are directional. As we have argued, because of the absence of commensurate energetic particles, conventional incoherent nuclear reactions cannot account for excess heat in the Fleischmann-Pons experiment, which is why we are interested in coherent processes. Coherent models in many cases show oscillatory behavior as does the example considered in this paper. We would have no problem in principle with a coherent process producing energy that shows oscillations.

However, in more sophisticated versions of the coherent models that we have studied, phonon loss in the vicinity of  $\omega_0$  must be included. In these models, the energy that is exchanged coherently with the oscillator thermalizes, which makes it unavailable for transferring back. So, even though the simple models that we focus on to begin the discussion do show oscillations, we agree with the reviewer that such oscillations should not occur in a realistic model for excess heat production. In the more sophisticated models that will be considered in later papers, thermalization of optical phonons results in unidirectional dynamics. For models describing excess heat. Some transfer of energy from the lattice (oscillator) to nuclear transitions however is predicted by our models, and has the potential to result in a lattice-induced X-ray or gamma-ray emission effect, independent of the Fleischmann–Pons experiment.

#### Appendix C.4. Limitations due to relativity

*The authors have not discussed issues associated with speed of light limitations in nuclear fusion, since the process is very fast (less than a femtosecond) once the deuterons get sufficiently close.*

Back in 1989, the notion was put forth that deuteron-deuteron fusion might be occurring in some new way, such that the reaction energy was somehow going directly into the lattice. Critics responded with the argument that once the deuterons got close enough to interact, the reaction itself was over long before there was time for communication with the nearest atoms.

We can quantify this argument starting with the reaction rate for molecular  $D_2$  written in the form

$$\gamma = A|\Psi(0)|^2,$$

where  $\Psi(r)$  is the molecular wavefunction for the relative deuteron separation;  $A$  is a reaction constant that is derived from the astrophysical  $S$  factor, and has a numerical value estimated to be [16]

$$A = 1.5 \times 10^{-16} \text{ cm}^3/\text{s}.$$

Hence, if we take the two deuterons to be localized within a spherical volume with maximum separation of  $r = 10$  fm

$$V = \frac{4\pi}{3}r^3 = 4.2 \times 10^{-36} \text{ cm}^3.$$

The associated reaction timescale given this localization could be estimated as

$$\tau = \frac{V}{A} = 2.8 \times 10^{-20} \text{ s}.$$

The associated speed of light limitation for this time interval is

$$c\tau = 8.4 \times 10^{-10} \text{ cm},$$

which is less than a tenth of an Angstrom. Critics used this argument effectively to convince others that it was impossible to couple energy to the lattice, since there was not sufficient time to communicate to the nearest atom that the reaction had occurred given the speed of light constraint.

We generally agree with this argument in connection with the incoherent fusion reaction process. The argument might be criticized in that there is some energy exchange with the lattice nonetheless since the lattice structure is changed instantaneously. We could compute the associated phonon exchange from existing theory; however, the effect is not large, and is unlikely to be measurable.

In the models that we have studied, the coherent energy exchange associated with the fractionation of a large nuclear quantum to optical phonons cannot be accomplished in the  $D_2/{}^4\text{He}$  system, since Coulomb repulsion makes the associated coupling strength much too small. Consequently, the picture that might be associated with this criticism is not one relevant to the models of interest to us.

#### Appendix C.5. Excitation transfer

However, some further discussion of the issue is worthwhile. In our earlier studies, we have considered  $D_2$  to  ${}^4\text{He}$  transitions mediated by phonon exchange, where the reaction energy is transferred elsewhere.

What we have termed excitation transfer as a physical effect has not been considered previously (outside of our work) in connection with nuclear reactions or MeV-level nuclear transitions. It is known in biophysics as the Förster effect, or as resonant energy transfer. An excited molecule can transfer its excitation to a nearby molecule through Coulomb dipole–dipole interactions. The effect is observed experimentally, and the theoretical explanation was given by Förster more than 60 years ago [17].

What we have proposed is that nuclear de-excitation can occur mediated by phonon exchange (rather than by Coulomb interactions), with the excitation energy being transferred to another nucleus (and subsequently coherently exchanged with the lattice). In this scenario, the issue raised by the reviewer then concerns whether this kind of de-excitation can occur in the presence of fast incoherent reaction rates. Since the coherent and incoherent processes are basically separate processes, one would address this by computing the rates for both processes; and if the rate associated with excitation transfer happens to be faster, then the answer would be yes. The situation in our models is made somewhat more complicated in that we need to consider the incoherent process as a loss mechanism in the coherent dynamics associated with the  $D_2$  to  ${}^4\text{He}$  transitions, but the essential argument is basically the same.

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