PROGRESS ON PHONON EXCHANGE MODELS FOR EXCESS HEAT IN METAL DEUTERIDES

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Abstract

Excess heat in the Fleischmann-Pons experiment without commensurate energetic particles implies a violation of local energy and momentum conservation. Models based on excitation transfer can produce a violation of local energy and momentum conservation under conditions where total energy and momentum are conserved. We present idealized spin-boson models that illustrate the excitation transfer mechanism. Spin-boson models also exhibit anomalous energy exchange, in which a large quantum is converted into many small quanta. We consider a model in which excitation transfer is followed by anomalous energy exchange, and we find an analytic solution for the coherent dynamics. The associated rates for the spin-boson models are too slow to be relevant to experiment. Spin-boson models augmented with oscillator loss show dramatically increased excitation transfer and anomalous energy exchange rates due to the elimination of destructive interference. The resulting rates can be comparable with experiment for reasonable assumptions about populations, matrix elements, and screening factors.

1. Introduction

The principal theoretical problem encountered in connection with the excess heat effect in the Fleischmann-Pons experiment [1] is the absence of energetic particles commensurate with the thermal energy produced. One foundation of nuclear physics is the conservation of local energy and momentum in scattering, decay, and reaction processes (a foundation which dates back to the time of Rutherford [2,3]). If local energy and momentum are conserved in an exothermic reaction, then the reaction energy must be expressed through energetic particles. In the Fleischmann-Pons experiment, an excess of energy is claimed, yet no experiment reported since 1989 has given any indication of energetic particles in amounts that would correspond to the energy produced.

Consequently, whatever physical process is responsible for the excess heat effect must violate local energy and momentum conservation if nuclear [4]. In 1989 the argument was made [1] that the energy produced was far too great to be of chemical or solid state origin, and hence must be nuclear through a process of elimination. No other kind of energy source was capable

in principle of the available energy density implied by the total energy release. Over the years a number of observations of ⁴He production have been reported, and in some cases where the total amount of ⁴He produced is correlated with the total excess energy measured. The reaction Q-value deduced from these experiments is near 24 MeV, which corresponds to the mass difference between two deuterons and ⁴He (see [5] and references therein).

These considerations provide some guidance as to what kind of new physical process should be sought in the development of a theoretical model. For example, the experimental results seem to provide support for reactions in which two deuterons interact in some new kind of way, such that ⁴He is made as a result. However, the absence of energetic particle production in association with the energy produced places severe constraints on what kinds of models may be relevant. For example, in previous years much energy was put into searches for anomalous screening effects, which might allow two deuterons to tunnel together more rapidly. Deuteron-deuteron fusion experiments at low beam energy have shown that very large anomalous screening effects are present in the case of a metal deuteride environment [6-8]. Nevertheless, such models do not address what is most important, which is the absence of energetic products. Anomalous screening by itself would lead to the production of energetic conventional deuteron-deuteron fusion products if strong enough; whereas experiments appear to show ⁴He (in the absence of 24 MeV gammas) with no commensurate energetic particles of any kind.

2. Excitation transfer

In response to this discussion, our attention should then focus on new physical processes in which local energy and momentum conservation is violated. Of course, minor violations of local energy and momentum conservation occur in the case of gamma absorption and emission is a solid, in which a small amount of momentum and energy is exchanged with the lattice in non-Mossbauer transitions. There is no possibility in our view of a new kind of process in which a large MeV-level quantum is exchanged with the lattice directly to produce a large number of low energy quanta.

The only real possibility for a violation of local energy and momentum conservation that remains is then through an excitation transfer process. We are not aware of any discussion of excitation transfer processes for excited states or reacting nuclei at a distance in the nuclear physics literature. However, excitation transfer is well known in biophysics [9,10]. In this case, atoms or molecules, which are distant, can exchange excitation through Coulomb coupling. Coupling between the two systems results in excitation transfer as a quantum coherent process, so that the interaction must be sufficiently strong to produce a transfer prior to decoherence of the entangled system. Unfortunately, Coulomb coupling falls off rapidly with distance, so that excitation transfer in atomic and molecular systems is limited to a short characteristic distance (the Forster length). There is no possibility of significant nuclear excitation transfer mediated through Coulomb coupling since the associated Forster length is very small.

2.1 Generalization of excitation transfer

If we adopt a more generalized view of excitation transfer, we might view excitation transfer as involving an off-resonant coupling between two equivalent two-level systems and extended

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ust violate ; made [1] and hence as capable common modes. For example, it is possible to analyze Coulomb coupling between dipoles mathematically in a picture in which each two-level system couples to common longitudinal photon modes. Since longitudinal photons have zero energy, the interaction is strongly offresonant, and intermediate states are produced with energies very different than the initial state energy. Destructive interference between the contributions of the different longitudinal photon modes then produces the spatial dependence associated with Coulomb coupling. Viewed this way, it is a relatively small step to a generalization of the effect where other modes are substituted in place of the longitudinal photon modes. For example, coupling to vibrational modes instead of longitudinal photon modes would produce a modified excitation transfer mechanism, with a different spatial dependence. The possibility of indirect coupling between two-level systems has been discussed in the literature [11]. Discussion of phononmediated indirect coupling has appeared in the solid state literature recently [12]. To extend such a model to the nuclear case requires phonon exchange in association with a nuclear transition. Aside from our interest in this problem, this seems not to have been explored in the literature previously outside of recoil effects associated with neutron capture and gamma transitions.

3. Idealized excitation transfer model

We can illustrate excitation transfer with the aid of an idealized model. Consider a pair of two-level systems that are coupled to a common oscillator, as described by the Hamiltonian

$$\hat{H} = \Delta E_1 \frac{\hat{s}_z^{(1)}}{\hbar} + \Delta E_2 \frac{\hat{s}_z^{(2)}}{\hbar} + \hbar \omega_0 \hat{a}^{\dagger} \hat{a} + V_1 (\hat{a}^{\dagger} + \hat{a}) \frac{2\hat{s}_x^{(1)}}{\hbar} + V_2 (\hat{a}^{\dagger} + \hat{a}) \frac{2\hat{s}_x^{(2)}}{\hbar}$$
(1)

Here, the components of the spin operator $\hat{s}^{(j)}$ for the two-level system j allow us to describe two individual two-level systems interacting with an oscillator (which is described by creation and annihilation operators \hat{a}^{\dagger} and \hat{a}). Coupling between the two-level systems and the oscillator is assumed to be proportional to the coupling coefficients V_1 and V_2 . We are interested in this problem in the limit in which the oscillator is highly excited, and where the oscillator energy $\hbar \omega_0$ is much less than the transition energies ΔE_1 and ΔE_2 . This model is a reduced version of the one discussed in [13] and in [14].

3.1 Energy levels and resonance condition

In this model, coupling between each two-level system and oscillator leads to an increase in the two-level transition energy, while the two-level systems have little impact on the oscillator. Energy levels are given approximately by

$$E_{n,m,m_2} = \Delta E_1(g_1)m_1 + \Delta E_2(g_2)m_2 + \hbar\omega_0 n$$

where the dimensionless coupling strengths g_1 and g_2 are given by

$$g_1 = \frac{V_1 \sqrt{n}}{\Delta E_1} \qquad g_2 = \frac{V_2 \sqrt{n}}{\Delta E_1}$$

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3.2 Dynamics

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The dressed transition energies are given approximately by [15]

$$\Delta E_{j}(g) = \frac{\Delta E_{j}}{\pi} \int_{\sqrt{\varepsilon}}^{\sqrt{\varepsilon}} \sqrt{\frac{1 + 8g^{2}y^{2}/n}{\varepsilon - y^{2}}} dy$$
(3)

with $\varepsilon = 2n+1$.

Excitation transfer may occur when two of these levels are degenerate. For example, when

$$\Delta E_2(g_2) - \Delta E_1(g_1) = \delta n\hbar\omega_0 \tag{4}$$

the dressed energy of the second two-level system matches the dressed energy of the first two-level system plus δn oscillator quanta. If δn is even, then the system can oscillate between two states in which excitation has been transferred from one system to the other (with some energy exchange with the oscillator).

3.2 Dynamics

On resonance, the system undergoes coherent Rabi oscillations between the two states, with dynamics given by

$$p(t) = \cos^2 \frac{|V|t}{\hbar} \tag{5}$$

where p(t) is the occupation probability of an initial state, with V the associated coupling matrix element. In an analytic WKB approximation this coupling matrix element is given approximately by

$$V = \frac{2\hbar\omega_0 g_1 g_2}{\pi n} \int_{\sqrt{\varepsilon}}^{\sqrt{\varepsilon}} \frac{1}{\sqrt{\varepsilon - y^2}} \frac{\cos\Delta\phi(y)}{\left[1 + 8\left(\frac{V_1 y}{\Delta E_1}\right)^2\right] \left[1 + 8\left(\frac{V_2 y}{\Delta E_2}\right)^2\right]} dy \tag{6}$$

where

$$\Delta\phi(y) = \frac{\Delta E_{1}}{\hbar\omega_{0}} \int_{0}^{y} \sqrt{\frac{1 + 8V_{1}^{2'}(y')^{2}/\Delta E_{1}^{2}}{\varepsilon - (y')^{2}}} dy' - \frac{\Delta E_{2}}{\hbar\omega_{0}} \int_{0}^{y} \sqrt{\frac{1 + 8V_{2}^{2}(y')^{2}/\Delta E_{2}^{2}}{\varepsilon - (y')^{2}}} dy' \quad (7)$$

Results are illustrated for a specific example in Figure 1.

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Figure 1: Level splittings $\Delta E_{\min} = 2|V|$ 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 $n_0 = 1000$. Results are presented for direct calculations with \hat{H} as given by Equation (1) at individual resonances – open circles; results from the WKB approximation – solid line. This calculation is discussed in [4].

3.3 Discussion

We draw attention to a number of features concerning this model and result. This model is the simplest possible that is capable of supporting an excitation transfer effect due to indirect coupling, and from the results we see that the effect is indeed present. We find that for significant excitation transfer to occur within the model, the resonance condition must be satisfied precisely, and the transfer rate observed is slow. We have found a rotation [13,15] which divides up the problem into an adiabatic piece, which is responsible for most of the level shift, and a dynamical piece, which is responsible for dynamical coupling between near resonant states. This allows us to treat excitation transfer coupling using a first-order matrix element even when multi-quantum transitions are involved.

We conclude that excitation transfer through off-resonant indirect coupling can arise in simple models involving coupling between two-level systems and an oscillator. Although the model is highly idealized, we have in mind applying the ideas in the case where the excited state of the first two-level system is a molecular D_2 at a site in a metal deuteride, and where the ground state is ⁴He located at the same site. The oscillator in this model stands in for a highly excited phonon mode that is common to both sites. The second two-level system represents the ground state and an excited state of a receiver nucleus. The excitation transfer process

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Once again the two-lev illustrated by the idealized model here is intended to shed some light on how excitation might be transferred from the D_2 upper state to another nucleus, leaving behind a ⁴He nucleus. Such a mechanism would violate local energy and momentum conservation in the D_2 /⁴He system, although overall energy and momentum conservation within the coupled oscillator and twosite nuclear system would be maintained. We note that in this kind of transfer process, the excitation energy is not transferred to the oscillator (in contrast to the assertions made by the reviewers at the 2004 DoE review). Unfortunately, the excitation transfer rates associated with this idealized model are much too slow to be relevant to excess heat production, so we will need to modify the model in some way to strengthen the effect.

4. Anomalous energy exchange

Were we to succeed in transferring the excitation from the $D_2/^4$ He system to produce excitation in a nucleus at another site, it would be reasonable to expect that this excited nucleus might decay, resulting in energetic charged particles as a consequence of local energy and momentum conservation. If so, then the system would proceed to express the reaction energy from the first site as energetic decay products from the second site, in contrast to observations. We might propose that another coherent excitation transfer process occurs prior to such an incoherent decay process, as we have in our previous ICCF conference proceedings papers. However, in such a proposal we still would not have faced up to the basic problem: we need to find a mechanism to dump the energy that does not involve decay via energetic particles. In our previous ICCF papers, we proposed that sequential excitation transfers from one site to another could eventually transfer energy to the oscillator, as long as a small amount of energy exchange occurred in association with each transfer process.

To shed light on this, we have studied idealized models for this effect, which we will term "anomalous energy exchange." As it turns out, the simplest version of the problem is one that is well studied in the literature, in the context of the Bloch-Siegert resonances [16] associated with the Rabi Hamiltonian [17] and spin-boson Hamiltonian [18]. In both models, one finds dynamical transitions directly between states in which one unit of two-level system excitation is exchanged for a large number of oscillator quanta. What is interesting in these models relative to our previous discussion is that excitation transfers from site to other sites are not required in order for the effect to occur. Only a single two-level system interacting with an oscillator is required.

5. Idealized model for anomalous energy exchange

The simplest model that exhibits the effect is the basic spin-boson model, given here by

$$\hat{H} = \Delta E \frac{\hat{s}_z}{\hbar} + \hbar \omega_0 \hat{a}^{\dagger} \hat{a} + V \left(\hat{a}^{\dagger} + \hat{a} \right) \frac{2\hat{s}_s}{\hbar}$$
(8)

Once again we are interested in the model when the oscillator energy $\hbar \omega_0$ is much less than the two-level system energy ΔE . The energy levels are given approximately by

$$E_{mn} = \Delta E(g)m + \hbar\omega_0 n \tag{9}$$

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$$\Delta E(g) = \Delta n\hbar\omega_0 \tag{10}$$

When this occurs, the system can undergo coherent Rabi oscillations between states in which a two-level system quantum is exchanged for many oscillator quanta.



Figure 2. Expectation values $\langle m \rangle$ and $\langle n - n_0 \rangle$ for an example in which the dressed two-level system energy $\Delta E(g)$ is matched to 25 $\hbar \omega_0$. Here, $\omega_0 = |U|/2\hbar$.

5.1 Dynamics

At resonance, the dynamics can be oscillatory with a probability for the system initialized in one of the resonant states given by

$$p(t) = \cos^2 \frac{|U|t}{\hbar} \tag{11}$$

where U is the associated coupling matrix element. This corresponds to the situation illustrated in Figure 2.

Figure 3. Energy strength g for the circles; WKB a nearly on top of

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Figure 3. Energy separation $E_{\min} = 2|U|$ at resonance as a function of the dimensionless coupling strength g for the case $\Delta E = 31\hbar\omega_0$ for $n = 10^8$. Exact results from solution of \hat{H} problem – solid circles; WKB approximation – open circles; analytic result – solid triangles. The WKB result lies nearly on top of the exact result. The rightmost resonance is for $\Delta E(g) = 85\hbar\omega_0$.

We have found that this coupling matrix can be approximated using an analytic WKB approximation as

$$U = i \frac{\hbar \omega_0}{\pi} \int_{\sqrt{\varepsilon}}^{\sqrt{\varepsilon}} \frac{\cos\left\{\frac{\Delta E}{\hbar \omega_0} \int_0^y \sqrt{\frac{1 + 8V^2 (y')^2 / \Delta E^2}{\varepsilon - (y')^2}} dy'\right\}}{1 + 8\left(\frac{Vy}{\Delta E}\right)} dy$$
(12)

where $\varepsilon = 2n+1$. This result is an analytic large *n* WKB approximation to the results discussed in [19]. In Figure 3 we show the level splitting at resonance from a direct calculation of the spin-boson Hamiltonian [Equation (8)], from a WKB approximation of the result discussed in [19], and from the analytic large *n* WKB approximation given here.

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5.2 Discussion

The basic spin-boson model exhibits an anomalous energy exchange something like what we need for describing excess heat in the Fleischmann-Pons experiment. To see the effect in the spin-boson model, a precise resonance must be present. In the rotated version of the problem, the multi-quantum transition can be described using a first-order coupling with a complicated matrix element, as discussed in [19]. This allows us to think of transitions where many quanta are exchanged in terms similar to that involving single quantum exchange.

The anomalous energy exchange effect itself in this model is relatively weak, requiring moderate to strong coupling, and producing a coherent rate that becomes slower the more quanta are exchanged. Although this kind of anomalous coupling qualitatively similar to what we need to convert an MeV quantum into a large number of low energy quanta, such models are simply not strong enough to lead to relevant conversion rates for the excess heat problem. Once again, we need to enhance the effect in order to develop models relevant to excess heat production.

6. Excitation transfer followed by anomalous energy exchange

In the discussion above, we see that very simple spin-boson models exhibit excitation transfer effects as well as anomalous energy coupling. Both are required to account for energy production without commensurate energetic particle emission in the Fleischmann-Pons experiment. The question arises then whether it is possible to develop a spin-boson type model which illustrates excitation transfer from one two-level system to another, followed by anomalous energy exchange between the second two-level system and the oscillator. Recognizing that the simple spin-boson models are too weak to account quantitatively for the excess heat effect, it is nevertheless interesting to develop such a model in the simpler system as we can obtain analytic solutions which can shed light on the mechanism under consideration.

6.1 Idealized model

Once again we consider a pair of two-level systems coupled to a common oscillator, using the same Hamiltonian as considered above:

$$\hat{H} = \Delta E_1 \frac{\hat{s}_z^{(1)}}{\hbar} + \Delta E_2 \frac{\hat{s}_z^{(2)}}{\hbar} + \hbar \omega_0 \hat{a}^{\dagger} \hat{a} + V_1 (\hat{a}^{\dagger} + \hat{a}) \frac{2\hat{s}_x^{(1)}}{\hbar} + V_2 (\hat{a}^{\dagger} + \hat{a}) \frac{2\hat{s}_x^{(2)}}{\hbar}$$

It is possible to select three states in the rotated version of the problem that are degenerate in the absence of the coupling responsible for excitation transfer and in the absence of coupling responsible for anomalous energy exchange [4]. The energy levels in this case are given approximately by

 $E_{n,m,m_2} = \Delta E_1(g_1)m_1 + \Delta E_2(g_2)m_2 + \hbar\omega_0 n$

6.2 Resonance

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6.2 Resonance conditions

We consider three states with energy eigenvalues in the rotated frame given by

$$E_{1} = \frac{\Delta E_{1}(g_{1})}{2} - \frac{\Delta E_{2}(g_{2})}{2} + \hbar \omega_{0} (n_{0} + \delta n)$$

$$E_{2} = \frac{\Delta E_{1}(g_{1})}{2} - \frac{\Delta E_{2}(g_{2})}{2} + \hbar \omega_{0} n_{0}$$

$$E_{3} = \frac{\Delta E_{1}(g_{1})}{2} - \frac{\Delta E_{2}(g_{2})}{2} + \hbar \omega_{0} (n_{0} + \Delta n)$$
(13)

A transition between the first state and the second state is an excitation transfer step in which the first two-level system is lowered and the second raised. This process is resonant when

$$\Delta E_2(g_2) = \Delta E_1(g_1) + \delta n\hbar \omega_0$$

A transition between the second state and the third state is an anomalous energy exchange step in which the second two-level excitation is exchanged for a large number of oscillator quanta. This process is resonant when

$$\Delta E_2(g_2) = \Delta n\hbar\omega_0$$

6.3 Dynamics

The system dynamics when both transitions are near resonance can be described using a three-state model of the form

$$p(t) = c_1(t)\phi_1 + c_2(t)\phi_2 + c_3(t)\phi_3$$
(14)

where the $c_i(t)$ are expansion coefficients, and where the ϕ_i are the basis states in the rotate frame that correspond to the three dressed energies given above. The dynamics are described by

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_1(t) \\ c_2(t) \\ c_3(t) \end{pmatrix} = \begin{pmatrix} E_1 & V_{12} & 0 \\ V_{21} & E_2 & V_{23} \\ 0 & V_{32} & E_3 \end{pmatrix} \begin{pmatrix} c_1(t) \\ c_2(t) \\ c_3(t) \end{pmatrix}$$
(15)

where the V_{jk} are matrix elements similar to those discussed in the previous sections.

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Figure 4. 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 (with probability p_2), only the second two-level system is excited; and in the third (with probability p_3), neither two-level system is excited. The frequency ω_0 in this case is $\sqrt{2}V/\hbar$.

In general, the three-state dynamics are very complicated, and we would spend much effort seeking to explain the significance. Perhaps more interesting to us in regard to this discussion is the special case in which the levels are degenerate and the coupling matrix elements equal in magnitude. In this special case, the resulting probabilities are given by

$$p_{1}(t) = \left[\frac{1 + \cos\left(\sqrt{2}|V|t/\hbar\right)}{2}\right]^{2}$$
$$p_{2}(t) = \left[\frac{\sin\left(\sqrt{2}|V|t/\hbar\right)}{\sqrt{2}}\right]^{2}$$
$$p_{3}(t) = \left[\frac{1 - \cos\left(\sqrt{2}|V|t/\hbar\right)}{2}\right]^{2}$$

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Results are illustrated in Figure 4 for this special case illustrating the analytic solutions. In this model, the system first undergoes an excitation transfer step, and then an energy exchange step. The associated dynamics are coherent throughout, and the system continues cycling back and forth between the three states periodically. This is discussed further in [4], in which model parameters are given for a specific case that was found to work this way.

6.2 Discussion

We have succeeded in developing idealized models based on spin-boson type Hamiltonians which exhibit coherent excitation transfer and anomalous energy exchange effects, similar to what is required for a description of the excess heat effect. In this model, the molecular D_2 state at a vacancy site inside the metal deuteride is represented by the upper state of the first two-level system, and the product ⁴He state at the same site is represented by the lower state. In this idealized model energy conversion itself occurs through the interaction of only a single receiver-side nucleus (as represented by the second two-level system) interacting with the oscillator. There are no site-to-site excitation transfers in this simplified model, yet efficient energy exchange occurs.

7. Loss

We have discussed previously that the augmentation of the idealized spin-boson models leads to a dramatic increase in the excitation transfer and anomalous energy exchange rates (for example, see [4]). The increase is sufficiently large that the resulting rates appear to be relevant to excess heat production.

7.1 Idealized model including loss and Dicke effects

The simplest model which includes these effects, along with Dicke enhancement effects, is given formally by the following Hamiltonian

$$\hat{H} = \Delta E_1 \frac{\hat{S}_z^{(1)}}{\hbar} + \Delta E_2 \frac{\hat{S}_z^{(2)}}{\hbar} + \hbar \omega_0 \hat{a}^{\dagger} \hat{a} - i \frac{\hbar}{2} \hat{\Gamma}(E) + V_1 \left(\hat{a}^{\dagger} + \hat{a} \right) \frac{2\hat{S}_x^{(1)}}{\hbar} + V_2 \left(\hat{a}^{\dagger} + \hat{a} \right) \frac{2\hat{S}_x^{(1)}}{\hbar}$$
(17)

Here, we consider matched sets of two-level systems (implemented through the manypseudospin operators \hat{S}_j , whereas we used single pseudospin operators \hat{s}_j above) for the donor (D₂/⁴He) two-level systems and receiver two-level systems. On the one hand, such a model includes new effects associated with sequential excitation transfer and anomalous energy exchange steps, which is of interest in addressing the production of macroscopic amounts of energy. On the other hand, this kind of model also describes cooperative effects between reactions at different sites, under the simplifying assumption that states and interactions at each site are equivalent.

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7.2 Implementation of loss

Included also in this model is a loss term $-i\hbar\hat{\Gamma}(E)/2$ that is intended to capture energetic decays associated with the oscillator (this is discussed more fully in [13]). It is reasonable to assume that the excited states of the two-level systems will have decay channels available. For example, the two deuterons can fuse to make energetic t+p and n+³He. One would expect decay channels to be accessible in excited states of receiver nuclei as well. However, neither of these processes impacts the excitation transfer and anomalous energy exchange rates, other than to damp both processes due to loss of excitation. It can be shown directly that the incoherent decay channels associated with the D₂/⁴He two-level system are not competitive with the coherent process under discussion, since the associated decay rates are unchanged from the situation in the absence of the coherent process (and are therefore very small). The situation on the receiver side is less clear at present, since much less is known from experiment about which nuclei and states are involved.

However, a different loss mechanism can have an enormous impact on the excitation transfer and anomalous energy exchange rates. If there occur strong loss channels for the oscillator in the vicinity of the two-level system transition energy, then the dynamics are altered fundamentally. An example of such a process might be a lattice-induced disintegration process, in which a constituent nucleus of the lattice fissions due in the course of transfer or exchange processes. The reason that the rates are impacted is because the rates for both processes are significantly reduced over the available coupling strength due to the interaction terms present in the Hamiltonian due to destructive interference effects. Oscillator loss channels can remove this interference, leading to a dramatic acceleration in both rates.

7.3 Interference effects in excitation transfer

The impact of loss on the destructive interference can be seen most readily in the case of excitation transfer in the weak coupling regime. In the case of excitation transfer between two individual two-level systems, six states contribute at lowest order in perturbation theory. There are initial and final states (states 1 and 6), in which the excitation of the two-level systems is switched, but where the oscillator excitation will be assumed unchanged. Then there are four off-resonant intermediate states in which both two-level systems are unexcited (states 2 and 3), or both excited (states 4 and 5), with oscillator excitation increased or decreased by one. If the intermediate states are eliminated, then the effective coupling between the initial and final states is [4]

$$V_{16}(E) = V_1 V_2 \left[\frac{n}{E - H_2 + i\hbar\Gamma/2} + \frac{n+1}{E - H_3 + i\hbar\Gamma/2} + \frac{n}{e - H_4} + \frac{n+1}{E - H_5} \right]$$
(18)

Since states 2 and 3 have energies much less than the available energy E, oscillator decay channels are accessible, which is reflected here by the appearance of loss terms associated with their contributions. Since states 4 and 5 have energies much greater than the available energy E, the oscillator decay channels are not accessible.

In the absence of loss ($\Gamma = 0$), strong interference occurs between the contributions from the different off-resonant states. In this case, the effective interaction reduces to

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$$V_{16}(E) \rightarrow \frac{V_1 V_2 \hbar \omega_0}{\left[\Delta E(g)\right]^2 - \left(\hbar \omega_0\right)^2} \quad \text{(no loss)} \tag{19}$$

This model can reproduce the excitation transfer results in the $\delta n = 0$ limit described earlier. On the other hand, if the loss is very strong, then the interference is removed. In the limit of infinite loss, the effective interaction becomes

$$V_{16}(E) \rightarrow \frac{2V_1 V_2 \Delta E(g) n}{\left[\Delta E(g)\right]^2 - \left(\hbar \omega_0\right)^2} \quad \text{(infinite loss)} \tag{20}$$

The effective interaction increases between these two limits by a factor of

$$\frac{\Delta E(g)}{\hbar \omega_0} n$$

This is an enormous effect. We see that the augmentation of the model with loss dramatically impacts the rate of excitation transfer.

7.4 Strong coupling limit

In [13] we examined the strong coupling limit of the lossy model, and developed estimates for dynamical rates. In light of the discussion above, it is perhaps not surprising that the maximum possible rates are closely associated with the interaction terms in the model.

For example, on the receiver side the maximum rate for phonon exchange is

$$\left[\frac{dn}{dt}\right]_{\max} = \frac{V_2 \sqrt{n}}{\hbar} \left(2\sqrt{S_2^2 - M_2^2}\right) \tag{21}$$

where S_2 and M_2 are receiver-side Dicke numbers. In essence, if there were only a single two-level system on the receiver side, this maximum anomalous energy transfer rate corresponds to the exchange of an oscillator quantum in association with each individual transition. If there are many receiver-side ground state nuclei, and only a few excited state receiver-side nuclei, then the rate will be proportional to the square root factor in the expression, which will evaluate roughly to the square root of the product of ground state and excited state nuclei of the receiver nuclei.

In the case of excitation transfer, the maximum rate depends on the coupling on both the donor side and the receiver side. However, since the donor side $(D_2/^4He)$ involves a hindered matrix element (since the Coulomb interaction produces a dramatic reduction in the overlap between the molecular D_2 state and the ⁴He state), it seems reasonable to examine the limit in which this part of the process is rate limiting. In this case, the maximum excitation transfer rate is

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$$\left[\frac{d\left(M_{1}-M_{2}\right)}{dt}\right]_{\max} = \frac{V_{1}\sqrt{n}}{\hbar} \left(4\sqrt{S_{1}^{2}-M_{1}^{2}}\right)$$
(22)

In essence, the model indicates that when loss is present, excitation transfer can proceed at the fastest rate that coherent transitions can occur. It is this rate which can be sufficiently fast to be relevant to excess heat production in the Fleischmann-Pons experiment.

8. Coupling matrix element

The evaluation and use of this model depends on the strength of the coupling between nuclei and phonons. We have recently developed a formalism with which detailed calculation can be made [20]. In that reference, we speculated that the coupling between molecular D_2 states and the ⁴He ground state could take place indirectly through n+³He channels. However, more recently we have found a direct coupling that will be dominant. A detailed calculation of this matrix element is in process, and will be reported on in the future. Nevertheless, some features have become apparent already in the process.

8.1 Compressional phonon mode interactions

It is clear that coupling occurs in the case of compressional phonon modes. Transverse phonon modes will participate only weakly if at all. This may be connected with observations by the ENEA Frascati group [21] that excess heat bursts resulting from laser stimulation occurs for TM polarization (which drive compressional surface plasmon modes [22]), and not for TE polarization. It may also be consistent with recent laser beating experiments reported by Letts et al [23], in which a response was observed at beat frequencies in the THz range within the optical phonon band, once again where TM polarization is required. At issue is the question of which modes are participating. Optical phonon modes would be advantageous for anomalous energy exchange since the frequency is greater; whereas excitation transfer could involve lower energy modes (there being no obvious requirement that both processes need be mediated by a single mode).

It seems clear also that the coupling will be strongest in the case of molecular D_2 S=2 (nuclear spin) states. This may have a connection with some experiments (such as [23]) in which the presence of a magnetic field seems to influence the effect.

8.2 Estimate and screening effects

Nevertheless, it is possible to estimate the interaction matrix element crudely based on elementary considerations. For example, the deuterons must tunnel through the Coulomb barrier to interact, so we expect a Gamow factor. Similarly, there is a significant volume change between localization of the deuterons in molecular D_2 and localization at the nuclear scale. Keeping these factors in mind, we would expect the matrix element to be on the order of

$$V_1 \sqrt{n} \to M_{fi} \quad \sqrt{\frac{v_{nuc}}{v_{mol}}} e^{-G_n}$$
 (23)

Here, M_{fi} i state and ' v_{mol} is the molecular barrier; the MeV.

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Here, M_{fi} is the matrix element for a strong-force mediated transition between a molecular D_2 state and ⁴He state involving phonon exchange; v_{nuc} is a characteristic nuclear volume and v_{mol} is the volume associated with the relative coordinate between the two-deuterons in the molecular D_2 state; *G* is the Gamow factor associated with tunneling through the Coulomb barrier; the parameter *u* is the residual interaction strength which is expected to be of order 1 MeV.

In the case of molecular D_2 in vacuum, this matrix element produces reaction rates at the femtowatt level or less for reasonable assumptions about the number of D_2 molecules that participate. Based on the beam experiments of [6-8] we know that screening is important in metal deuterides. In [13] we estimated that a screening energy of about 115 eV would be required to obtain agreement between this model and excess power in the Fleischmann-Pons experiment, assuming that the molecular D_2 species were constrained to be in the outer part of the cathode at sites with single host atom vacancies.

9. Conclusions

Any explanation of excess heat in the Fleischmann-Pons experiment must confront the absence of energetic particles commensurate with excess energy production. The implication is that whatever process is responsible for excess heat violates local energy and momentum conservation. The experimental observation of ⁴He as an ash with a reaction *Q*-value of 24 MeV points toward reaction mechanisms involving deuteron-deuteron interactions that result in ⁴He. Based on these considerations, we have proposed and studied reaction mechanisms in which excitation transfer stabilizes ⁴He at the initial reaction site (violating local energy and momentum conservation), with the large energy quantum of the reaction converted to lower energy quanta through anomalous energy exchange.

We have examined idealized spin-boson models to illustrate the off-resonant excitation transfer and anomalous energy exchange effects. The simplest possible models that could possibly exhibit such effects show them clearly, as we have presented here. It is possible to develop spin-boson type models in which excitation transfer is followed by matched anomalous energy exchange, in which we can solve analytically for the associated coherent dynamics. These models make clear that the required mechanisms exist and can be studied independently or together at our leisure. The associated dynamics in these examples is coherent, and we are able to treat excitation transfer and anomalous energy exchange through moderately complicated first-order matrix elements in a rotated version of the problem.

Although we learn much from the idealized models, they are simply not strong enough to account for the excess heat effect, since the associated dynamical rates are too slow. The reason that the rates are slow is that destructive interference occurs in both cases. Models that include oscillator loss at the two-level transition energy have greatly enhanced rates of both excitation transfer and anomalous energy exchange due to the elimination of this destructive interference. Such models are capable of predicting reaction rates in the range of observations based on crude estimates for the coupling matrix element, given significant screening (but screening which is modest in comparison to low energy deuteron-deuteron fusion experiments at low energy).

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