

# **Excitation transfer and energy exchange processes for modeling the Fleischmann-Pons excess heat effect**

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## **Abstract**

The absence of energetic particles commensurate with the energy produced is the single most notable feature of the Fleischmann-Pons experiment for theory, assuming that a new nuclear process is involved. We discuss briefly energy exchange between two-level systems and a low energy oscillator, concluding that spin-boson models augmented with loss are able to describe coherent energy exchange involving a large number of oscillator quanta. Since the coupling between deuterons and the lattice is weak, the excitation must be transferred to a different system with stronger coupling, in order to develop a simple model relevant for heat production. The resulting toy model can be used for simulation, and we describe briefly ongoing efforts to develop a computational model.

## **Introduction**

The Fleischmann-Pons effect consists of excess heat production in experiments where palladium cathodes are electrolyzed in heavy water; the amount of energy measured in such experiments is much too large to be of chemical origin; and energetic particles commensurate with the energy produced are absent. When first described in 1989, the response of the scientific community was one of skepticism and disbelief. Early efforts to confirm the effect were largely unsuccessful, due to a lack of understanding as to what are the critical issues. Subsequent experimental work in the following years has provided enough confirmations that the effect is at present held to be real among researchers who work in the area.

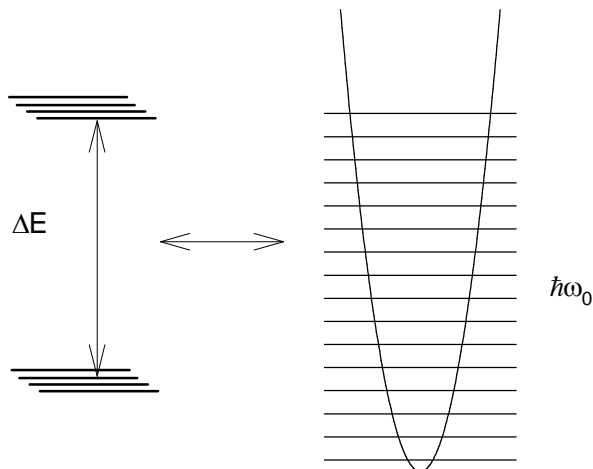
There is at present no accepted theoretical explanation for the effect. Since the inception of nuclear physics in the early 20<sup>th</sup> century, nuclear reactions have been understood in part through the concept of local energy and momentum conservation. In an exothermic nuclear reaction, the net energy produced is expressed in terms of energetic particles. No nuclear reactions are known in which most of the energy produced goes into other channels.

However, this foundation of nuclear physics is precisely what is challenged in the Fleischmann-Pons experiment. Hence, the primary theoretical focus, if one accepts that the energy is of nuclear origin and that commensurate energetic particles are not present, must be on physical mechanisms that lead to a violation of local energy and momentum conservation (while conserving overall momentum and energy).

## Energy exchange

There is some experimental support for a reaction Q-value of 24 MeV per  $^4\text{He}$  atom observed in the gas phase, in experiments where an effort was made to scrub the helium out of the cathode [1,2]. This directs our attention to mechanisms in which two deuterons (as fuel) combine to make  $^4\text{He}$  (as ash), where the mass difference (24 MeV) is to be converted to a very large number of lower energy quanta. Experiments have been reported recently in which cathodes have been observed to respond to laser beat frequencies at 8 THz and 15 THz (and also 20 THz), which correspond to the optical phonon band edges of PdD (and also PdH) [3]; these are modes with zero group velocity. This motivates us to consider optical phonon modes as oscillator modes involved in the energy exchange process.

The theoretical problem to be addressed, then, is how a large energy (24 MeV) quantum can be split up efficiently into a very large number of small energy (33 or 62 meV) quanta. We have studied models in which two-level systems with a large transition energy (representing local molecular  $\text{D}_2$  and  $^4\text{He}$  states at vacancy sites in the PdD lattice) couple to a low energy harmonic oscillator (representing optical phonon modes with low group velocity). Such models at first glance appear to be closely related to spin-boson models that appear in the literature in connection with NMR, cavity QED, and other applications. When a two-level system is coupled to an oscillator with much lower characteristic energy, then the models predict that energy can be exchanged between the two systems. For this to occur, the resonance must be very precise, and the resulting energy exchange rate is very slow. In the end, one would not expect to see more than about 100 oscillator quanta exchanged for a two-level system quanta, due to the weakness of the energy exchange effect in the multi-quanta limit.



**Figure 1:** Two-level systems coupled to a harmonic oscillator, in a many-spin spin-boson model.

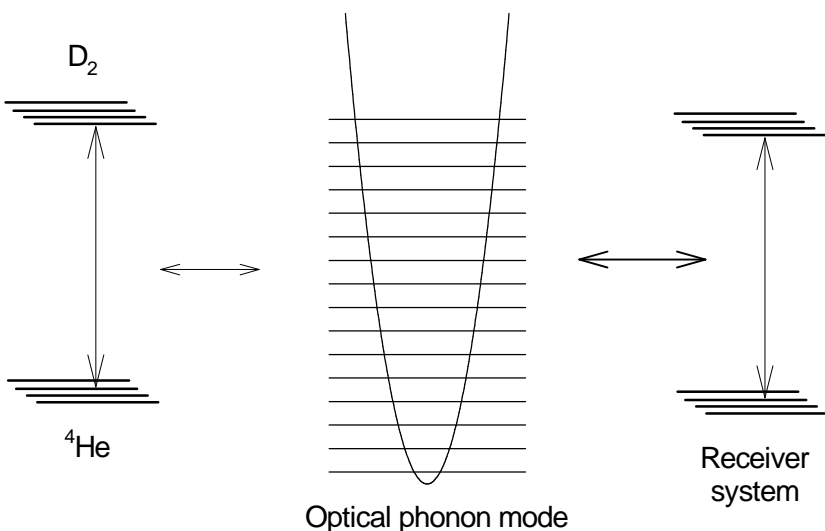
However, if we examine the many-spin version of the spin-boson problem, we find that energy exchange is hindered by destructive interference effects between the different individual pathways involved. If this destructive interference is spoiled, then the rate of energy exchange is greatly enhanced, and the number of oscillator quanta that can be exchanged with a two-level system is increased dramatically. Spin-boson models augmented with loss exhibit greatly increased energy exchange rates. An example of this is discussed in the Appendix. Such models allow energy exchange between low energy oscillators and energetic two-level systems that is

sufficiently rapid to account for the kind of energy exchange required in Fleischmann-Pons experiments, at least in principle.

## Excitation transfer

The use of spin-boson models requires an estimate for the coupling matrix elements between the two-level system and the oscillator. To apply this kind of model to describe nuclear transitions involving phonon exchange, we require an estimate for the associated matrix element. There is no difficulty in principle with a direct computation of the matrix element between molecular  $D_2$  and nuclear  $^4He$  states in the lattice, including phonon exchange [4]. However, we know that this matrix element is small due to the presence of a Gamow factor associated with tunneling through the Coulomb barrier. Many-spin spin-boson models augmented with loss require the coupling to be strong in order for the energy exchange process described above to function. As a result, the simplest possible models for energy exchange cannot work in the case of direct transitions between  $D_2$  and  $^4He$ .

Consequently, we seek a modification of this basic model. In recent years we have focused on models involving two different sets of two-level systems, both coupled to a common oscillator. One of these sets of two-level systems is strongly coupled to the oscillator, and the other is assumed to be weakly coupled to the oscillator. The basic idea in this kind of model is that the excitation associated with the weakly-coupled two-level systems is transferred over to the strongly-coupled two-level systems, where many-quantum energy exchange can occur [5]. This is indicated schematically in Figure 2.



**Figure 2:** The  $D_2/{}^4He$  system (modeled as a set of equivalent two-level systems) is weakly coupled to a low energy oscillator. A second set of two-level systems (indicated as the receiver system) is strongly coupled to the oscillator.

Computations done to date indicates that the basic scheme seems up to the task of modeling the Fleischmann-Pons excess heat effect, as long as the associated many-spin model is augmented with loss (which greatly accelerates the excitation transfer process as well as the energy exchange process). The enhanced excitation transfer rate is sufficiently fast in the case of the weak coupling matrix element associated with the  $D_2$ - ${}^4He$  transition to be consistent with experiment (as long as substantial screening effects comparable to those estimated by Cserki and coworkers [6] for PdD are included).

However, input from experiment does not tell us what the relevant physical states are that correspond to the strongly-coupled two-level system on the receiver side. There are at least two plausible candidates which seem to have theoretical support and are not inconsistent with experiment:

One possibility is that nuclear states of the host lattice participate. In this case, the ground state of the two-level system would correspond to the ground state of neutron rich isotopes of the host (such as  $^{110}\text{Pd}$ ). The upper state would correspond to an exotic nuclear state in which a neutral cluster (such as  $^4\text{n}$ ) separated from the daughter nucleus ( $^{106}\text{Pd}$ ) by about 10 fm, perhaps with some angular momentum. Such a state would be favored by the selection rules associated with coupling to the lattice (phonon exchange in association with nuclear excitation in general seems to be a weak effect, that becomes much stronger in the event that the lattice “sees” a mass change of the nucleus). Whether this kind of state can be sufficiently stable to do what is required within the context of the model has not been demonstrated.

Another possibility is that nuclear states similar to those of the  $\text{D}_2\text{-}^4\text{He}$  two-level systems participate. In this case, the  $^4\text{He}$  ground state would match the ground state of the receiver-side two-level systems. The excited state in this scenario would be a compact molecular  $\text{D}_2$  state, formed by a competition between production (where the source involves creation at fermi-level separation) and destruction (where transitions back down to the ground state occur sufficiently rapidly to prevent  $\text{D}_2$  separation out to 0.74 Angstroms). As long as the reduced  $\text{D}_2$  separation was sufficiently large so that the difference in the electronic wavefunctions is significant (ultimately leading to phonon exchange), and conventional fusion pathways occurred sufficiently slowly so as not to drain off the excitation, then such a state would be able to fulfill the functional requirements of the model.

## Simulation model

The development of an idealized microscopic model for excitation transfer and energy exchange allows us to consider using it in the context of a simulation model. A picture has been in the process of emerging over a great many years which seems to be consistent with many experiments, and which seems to be consistent with the requirements of the microscopic model.

In this picture, deuterium is loaded into Pd so that the associated chemical potential becomes high enough to support vacancy stabilization (which occurs near a D/Pd ratio of 0.94). At this loading, Pd that is codeposited will have a large number of single-atom vacancies. There is the possibility that vacancies can diffuse from the outer surface, but the associated kinetics are expected to be slow unless there exists an enhancement under conditions where a deuterium flux is present. In the basic Fleischmann-Pons experiment, the formation of the vacancies is thought to require about a month (and a much shorter time in the Szpak experiment). The loading and vacancy stabilization can be simulated from information available in the literature; to model the surface vacancy distribution requires knowledge of the rate of codeposition, or enhanced vacancy diffusion rates.

We conjecture that  $\sigma$ -bonded dideuterium [7] (essentially molecular  $\text{D}_2$ ) forms in the vacancies at more modest loadings. These are the active sites, which occur in the outer (micron-scale) region of the cathode. Dideuterium formation can be modeled using simple statistical mechanics given an estimate of the binding energy. Excitation transfer is then stimulated by phonon exchange with compressional phonon modes (the matrix element between  $\text{D}_2$  and  $^4\text{He}$  couples

predominantly to compressional phonon modes) that are highly excited. Phonon excitation in this picture is produced by the deuterium flux through the near-surface of the cathode. Energy exchange occurs in the presence of high compressional optical phonon excitation in the case of assumed  $^4\text{He}$ -compact  $\text{D}_2$  states (which at present seems to match experiment best). The simplified model described above consisting of two-sets of two-level systems to account for the nuclear states, and a harmonic oscillator (augmented with loss) to model optical phonon modes, can be used to develop equations describing the associated coherent dynamics for the simulation model.

As energy is produced,  $^4\text{He}$  accumulates in the active sites. At first, this would be helpful as there would be more capacity for anomalous energy exchange, since in general there is little helium present initially. However, as more energy is produced, we expect helium to block active sites, since the diffusion of helium away from the active sites is very slow near room temperature. In the event that helium diffusion limits excess heat production, we would expect to see a strong temperature dependence associated with excess heat production (as has been reported in a number of experiments [8]). With an appropriate simulation model, we can model this effect, and compute the fraction of helium released into the gas.

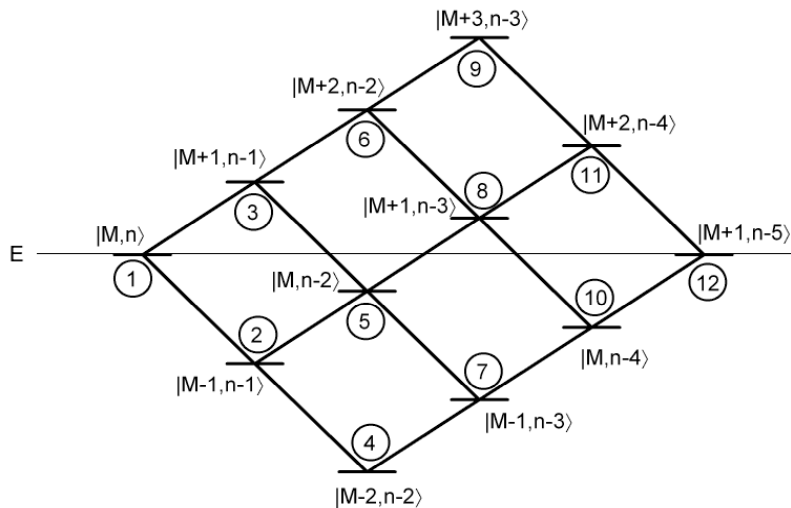
We have begun the development of the simulation model outlined above. The results obtained so far seem to be interesting, and we hope to compare our results with experiment in the coming months.

## Appendix

Consider the enhancement of multi-quantum coherent energy exchange in a many-spin spin-boson model augmented with loss. We take the Hamiltonian to be of the form

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

Where the first term in the Hamiltonian describes the energy of the two-level systems, the second term describes the oscillator, the third term implements linear coupling, and the final term accounts for the loss added to the model. The model is discussed further in [9].



**Figure 3:** Energy levels that contribute to indirect coupling between  $|M,n\rangle$  and  $|M+1,n-5\rangle$  in the case of multi-quantum exchange involving 5 quanta.

The impact of loss on energy exchange can be illustrated through a concrete example. We consider a finite basis solution constructed from a combination of 12 basis states composed individually of products of Dicke states and oscillator states

$$\Psi = \sum_j c_j |S, M_j\rangle |n_j\rangle$$

We consider indirect coupling from an initial state  $|M, n\rangle$  to a final state  $|M+1, n-5\rangle$ , in which a single two-level system excitation is matched to a loss of 5 oscillator quanta. The states are illustrated in Figure 3.

If no loss is present, the indirect matrix element between the initial state and the final state can be found to lowest-order in perturbation theory to be

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

If loss is present and large for all intermediate states with a basis energy less than  $E$ , such that the associated paths do not contribute, then the indirect coupling matrix element is

$$V_{1,12} = \frac{1}{18} \left[ 5S^4 + 10S^3 - S^2(10M^2 - 8M - 22) + \cdots \right] [V_{1,12}]_{\Gamma=0} \quad \Gamma \rightarrow \infty$$

For modest  $S$  the enhancement in indirect coupling is orders of magnitude. Loss breaks the destructive interference between the contributions from different pathways, and results in a dramatic increase in the indirect coupling responsible for coherent multi-quantum energy exchange.

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