LATTICE-INDUCED ATOMIC AND NUCLEAR REACTIONS

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ABSTRACT

A new theory for a variety of atomic and nuclear reaction mechanisms resulting from the decay of a highly excited lattice is introduced.

In our previous work on neutron transfer reactions, we found that large energy transfer between a lattice and nuclei could occur through the frequency shift of a highly excited continuum phonon mode across a band gap that is caused by the neutron transfer. Here, we generalize the energy transfer mechanism to include impurity continuum phonon modes due to the presence of vacancies; processes that change the number of vacancies can in principle stimulate the transfer of energy with the lattice.

A consequence of this is that a metal hydride lattice with host vacancies that has very high excitation of gap-jumping phonon modes will be unstable against decay by a variety of atomic and nuclear processes. Coulomb-induced recoil reactions of nuclei with electrons and nearby nuclei that cause vacancy production are found to occur with very high predicted reaction rates.

A lattice with a large number of highly excited phonon modes that can decay sequentially will most likely decay with a "burst" of emitted decay products, as a high order multi-step quantum process. A theory for this type of high-order decay is outlined.

The predictions of this theory may apply to many of the anomalous phenomena claimed to occur in experiments performed on metal deuterides, including neutron production, tritium production, gamma emission and host lattice activation.

1. Introduction

Nearly five years have passed sinced the initial announcement by Pons and Fleischmann[1] of the observation of what they and others have termed "cold fusion." During this time, a wide variety

of claims have been made for the observation of anomalous phenomena of one sort or another in PdD, in TiD_2,[2–5] in other metal deuterides,[6,7] and now also in metal hydrides.[8–10] Perhaps most important, if true, is the claimed observation of excess heat; the heat production reported is sufficiently large that if real, it would not be attributable to chemical or other atomic effects.[11] Many in the field hope that this effect, believed to be due to yet unknown nuclear reactions, will eventually be harnessed to provide a new clean source of energy for mankind.

The scientific community has long since grown immune to any reports of such claims. In a sense, the field of "cold fusion" has been judged, the data weighed and found wanting, and the field sentenced to oblivion. The cause: experiments that seem not to be reproducible, data that may suffer from either systematic errors or poor signal to noise ratio, no consistent effect that appears in all experiments, and no compelling theoretical reason to believe that anything anomalous should happen at all. No obvious progress has been made during the past year in effecting a basic change in attitude.

Our research in the area takes as its premise the possibility that some of the experimental results are in fact correct, and seeks to address the question as to what physical mechanisms, if any, could be responsible. Our studies have led us to consider numerous potential nuclear reaction pathways, focussing on possible enhancements in reaction rates that might be brought about by the atomic environment. Due to the large energy required to cause anything nuclear to happen, it is crucial in any such candidate theory for a clear and obvious energy transfer mechanism to be present that is capable of transferring such large energy.

Recently, such a mechanism was identified in the case of reactions that involve neutron transfer.[12] The basic idea is to generate a very large number of phonons into a small number of continuum phonon modes, and then shift the frequency of these phonon modes by transferring a neutron to or from a nucleus in the lattice. The total energy transfer through this mechanisms is

$$\Delta E = n\hbar\delta\omega \tag{1.1}$$

where $\delta\omega$ is the frequency shift, and where where n is the number of phonons present in the frequency-shifting modes.

To arrange for a continuum phonon mode to change its resonant frequency can be accomplished in certain materials that possess an impurity phonon band separated from other phonon modes by a finite band gap; a neutron transfer process that changes the number of impurity atoms also causes a change in the number of impurity phonon modes, which implies that a small number of phonon modes must jump the band gap. To arrange for a large number of phonons to be in a small number of phonon modes essentially implies the presence of a phonon laser.

Recently we have proposed the generalization of this mechanism to a much wider class of processes, some of which are nuclear and some of which are atomic. The key observation is that an impurity band can be due to the presence of vacancies, which implies that mechanisms that alter the number of vacancies of a certain type can in principle cause a large energy transfer to occur.

For example, in a metal deuteride that possesses a large band gap between the acoustic and optical phonon branches, it may occur that impurity bands for those deuterium atoms near a vacancy will form within the band gap. In PdH, for example, the basic hydrogen occupation of octohedral sites persists in lattice cells with a Pd vacancy;[13] we assume that the same is true in PdD. Deuterium atoms next to a Pd vacancy see a softer potential, and consequently oscillate at a lower frequency, than deuterium atoms not next to a vacancy. The frequency of this type of defect vacancy band is presently unknown; we will make the anzatz in this work that these modes in fact lie within the band gap in the case of the metal deuteride PdD (see Figure 1). A change in the number of vacancies will result in a change in the number of vacancy phonon modes; new vacancy modes are formed from the lowest modes above the band gap, which jump down to join the vacancy impurity band.

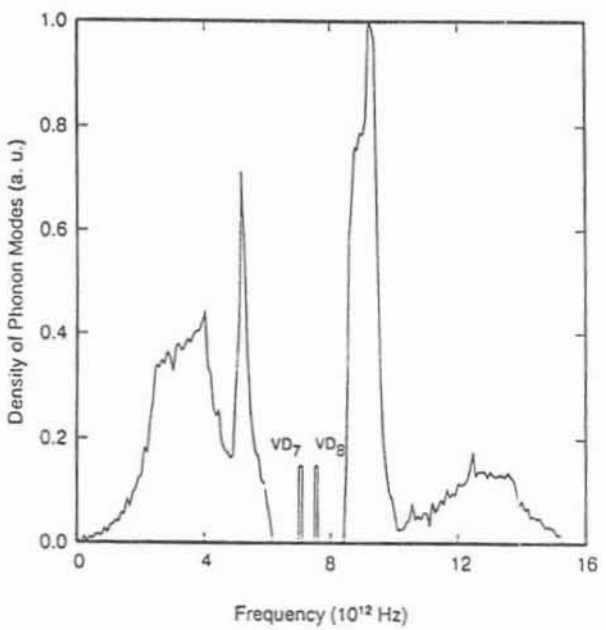

Figure 1: Density of states in PdD (based on the force constants of Ref. 14), augmented with proposed vacancy impurity bands (VD_7 and VD_8). VD_8 indicates modes due to cells with 8 deuterons around a Pd vacancy; VD_7 indicates modes due to 7 deuterons around a Pd vacancy.

In a metal hydride that works in the way outlined above, the generation of a very large number of

phonons in "gap-jumping" phonon modes results in an unstable system that will decay through any mechanism that produces an additional vacancy. For example, the Coulomb interaction between an electron and a nucleus can result in a fast ejected electron, as long as the recoil is sufficient to irreversibly displace the nucleus; in this case the reaction energy is supplied by the lattice through frequency-shifting a large number of phonons, which is caused by the reaction. Coulomb interactions between neighboring nuclei can cause recoil capable at lower energy of ejecting nuclei and causing phonon mode jumps. In the event that the lattice transfers a very large amount of energy, nuclear decay channels become available.

In what follows, we will outline briefly the basic theory for anomlous energy transfer from the lattice, and then review results for various decay channels. Although it is straightforward to compute reaction rates using Fermi's Golden Rule, we find that the rates predicted in this way are much too large for the processes to occur independently; Fermi's Golden Rule breaks down. Consequently, if the processes occur at all, they must occur in bursts as coupled reactions. The generalization of the theory to describe coupled reactions is straightforward formally, but leads to formulas for reaction rates that appear to be difficult to evaluate; we propose a method to extract numerical results from these formula.

2. Lattice-Induced Fast Electron Production

The decay of a highly-excited atomic or nuclear system by Coulomb-mediated fast electron production is well known: in the atomic system the process is known as autoionization, or Auger decay; in the nuclear system, this process is known as internal conversion. A molecule with a very high level of vibrational excitation could in principle decay through electron ejection, although the author is not aware of any examples where this has been observed. The decay of a highly excited lattice by fast electron ejection as a direct process has not been described previously.

A lattice with a highly-excited gap-jumping mode will be able to decay by electron ejection, as long the recoil is sufficiently great for a vacancy to be produced. As an example, we consider lattice decay through ejection of a K-shell electron, in a lattice with very great excitation of the lowest optical phonon modes. The electron recoil in this case must be sufficiently strong to permanently dislodge the nucleus. Our goal in what follows here is to describe a theory for this process that includes explicitly the energy transfer from the lattice, the Coulomb interaction between electron and nucleus, and the resulting nuclear recoil.

In perhaps the simplest possible model for such a decay process, we may start with Fermi's Golden Rule

$$\Gamma = \frac{2\pi}{\hbar} \sum_f \sum_{\mathbf{k}} | < \Psi_i | \hat{V} | \Psi_f > |^2 \delta(I_K + \hbar^2 |\mathbf{k}|^2 / 2m_e + E_f^{(L)} - E_i^{(L)}) \tag{2.1}$$

In this formula, the phonon operator $\hat{V}$ is the Coulomb potential between the nuclei and the K-shell electrons

$$\hat{V} = \sum_j \sum_{j'} \frac{Ze^2}{|\mathbf{r}_{j'} - \hat{\mathbf{R}}_j|} \tag{2.2}$$

where $\mathbf{r}$ refers to the electron coordinate, and where the nuclear center of mass coordinates $\hat{\mathbf{R}}_j$ are taken to be lattice phonon operators. The summations are over all final lattice states f and final electron momenta $\mathbf{k}$. Energy conservation is constrained between the initial lattice energy and final lattice plus electron energy; I_K is the K-shell electron binding energy.

The individual matrix elements that occur in the Fermi's Golden Rule rate formula

$$M = < \Psi_i | \hat{V} | \Psi_f > \tag{2.3}$$

approximately factor into parts that can be individually identified with Coulomb exchange, recoil and mode frequency-shifting, as we will argue below. To do so, we will use the Born approximation for the free electron, and the Born-Oppenheimer approximation for the lattice nuclear motion.

For the computation of an individual matrix element, the initial and final state wavefunctions are taken to be product wavefunctions that are built up from lattice wavefunctions $\Psi^{(L)}$ and single electron orbitals ϕ as follows:

$$\Psi_i = \Psi_i^{(L)} \phi_{1s}(\mathbf{r} - \hat{\mathbf{R}}_j) \tag{2.4}$$

$$\Psi_f = \Psi_f^{(L)} \phi_{\mathbf{k}}(\mathbf{r}) \tag{2.5}$$

This form of initial and final state wavefunctions is appropriate for a rate involving a single electron transfer; had we started with a more complicated many-electron wavefunction, we would find that only one orbital at a time contributes to the total rate. We must keep the total lattice wavefunction at this point, since the vibrational energy that is transferred in the process is not localized.

The integration over an electron coordinate at site j yields

$$\int \phi_{1s}^*(\mathbf{r} - \mathbf{R}_j) \frac{Ze^2}{|\mathbf{r} - \hat{\mathbf{R}}_j|} \varphi_{\mathbf{k}}(\mathbf{r}) d^3\mathbf{r} = V(\mathbf{k}) e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_j} \tag{2.6}$$

where

$$V(\mathbf{k}) = Ze^2 \left[\frac{N_{1s}}{V}\right]^{\frac{1}{2}} \left[\frac{Z^3}{\pi a_0^3}\right]^{\frac{1}{2}} \frac{4\pi}{|\mathbf{k}|^2 + (Z/a_0)^2} \tag{2.7}$$

assuming a nonrelativistic $1s$ hydrogenic orbital and a plane-wave $e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$ continuum orbital; the number of $1s$ electrons in the K-shell orbital at site j is N_{1s}.

The matrix element for a Coulomb exchange that occurs at site j can now be written as

$$M = V(\mathbf{k}) < \Psi_i^{(L)} | e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_j} | \Psi_f^{(L)} > \tag{2.8}$$

The definitions of the phonon modes may differ between the initial and final lattice states, so that some care must be taken in analyzing this matrix element. In our previous work on energy transfer in the case of neutron capture reactions,[15] we found that correct answers could be obtained most simply by taking equation (2.8) to be defined as involving integrations over nuclear center of mass coordinates

$$M = V(\mathbf{k}) < \Psi_i^{(L)}(\{\mathbf{R}\}) | e^{i\mathbf{k}\cdot\mathbf{R}_j} | \Psi_f^{(L)}(\{\mathbf{R}\}) > \tag{2.9}$$

temporarily dispensing with carats to indicate phonon operators. Considering all terms to be functions of center of mass coordinates removes any such problems because the center of mass coordinates themselves are invariant during Coulomb exchange. The nuclear center of mass coordinates can be expressed in terms of the initial state and final state phonon mode amplitudes q_m through

$$\mathbf{R}_j = \mathbf{R}_j^{0,i} + \sum_m \mathbf{u}_m^{(i)}(j) q_m \tag{2.10}$$

$$\mathbf{R}_j = \mathbf{R}_j^{0,f} + \sum_m \mathbf{u}_m^{(f)}(j) q_m \tag{2.11}$$

where $\mathbf{u}_m^{(i)}(j)$ and $\mathbf{u}_m^{(f)}(j)$ are the lattice displacement vectors for the initial and final lattices.

We need to recast the matrix element M in terms of phonon mode amplitudes in order to analyze frequency-shifting effects. Changing over to phonon amplitudes leads to

$$M = V(\mathbf{k}) C < \Psi_i^{(L)}(\mathbf{q}_i) | e^{i\mathbf{k}\cdot\mathbf{R}_j} | \Psi_f^{(L)}(\mathbf{q}_f) > \tag{2.12}$$

The normalization coefficient C is required since the initial and final state phonon amplitudes may not be equivalent. Due to this inequivalence, the matrix element is very difficult to compute in its present form: we would be able to make further progress if we could express Ψ_f in terms of $\mathbf{q}_i$.

As a consequence of the invariance of the center of mass coordinates during Coulomb exchange, there exists a linear relationship between the initial and final state mode amplitudes. From equations (2.10) and (2.11), it is possible to compute individual final state phonon amplitudes in terms of initial state phonon amplitudes; the resulting relation can be summarized as

$$\mathbf{q}_f = \mathbf{A} \cdot \mathbf{q}_i + \mathbf{b} \tag{2.13}$$

in the case of a harmonic lattice. This problem is well known in the case of electronic transitions in polyatomic molecules, and the above relation between initial and final state phonon amplitudes is called a Duschinsky transformation.[16]

Our goal of obtaining the final state wavefunction in terms of the initial state coordinates is accomplished through the use of the Duschinsky operator $e^{-i\hat{S}_D}$,[17] which has the property

$$e^{-i\hat{S}_D}\psi(\mathbf{q}_i) = \psi(\mathbf{A} \cdot \mathbf{q}_i + \mathbf{b}) = \psi(\mathbf{q}_f) \tag{2.14}$$

We may use this to rewrite the matrix element M as

$$M = V(\mathbf{k}) < \Psi_i^{(L)}(\mathbf{q}_i)|e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_j}e^{-i\hat{S}_D}|\Psi_f^{(L)}(\mathbf{q}_i) > \tag{2.15}$$

once again using carats to indicate phonon operators.

There exists a very large number of phonon modes in a macroscopic lattice, but only a few modes can undergo a significant frequency shift during the creation of a single vacancy. Although the frequency-shifting modes will be involved in the recoil, recoil effects will be dominated by the vast majority of the modes that do not undergo any significant frequency shift. This suggests that a separation between recoil effects and frequency-shifting would be a reasonably good approximation, leading to

$$M \approx V(\mathbf{k}) < \Psi_i^{(L)}(\mathbf{q}_i)|e^{-i\hat{S}_D}|\Psi_f^{(L)}(\mathbf{q}_i) >_{m^*} < \Psi_i^{(L)}(\mathbf{q}_i)|e^{i\mathbf{k}\cdot\mathbf{R}_j}|\Psi_f^{(L)}(\mathbf{q}_i) >_m \tag{2.16}$$

where $< \cdots >_m^*$ denotes an average over the gap-jumping modes, and where $< \cdots >_m$ denotes an average over non gap-jumping modes. This result perhaps exhibits most cleanly the physics involved in the proposed decay of a highly excited lattice by electron emission: the Coulomb exchange between nucleus and electron results in $V(\mathbf{k})$; energy transfer of the lattice comes about through frequency shifts in a small number of phonon modes; and the vacancy production required for energy transfer to occur is a simple recoil effect.

The reaction rate for a transition at site j is then given by

$$\Gamma_j = \frac{2\pi}{\hbar}\sum_f\sum_{\mathbf{k}}|V(\mathbf{k})|^2| < \Psi_i^{(L)}(\mathbf{q}_i)|e^{-i\hat{S}_D}|\Psi_f^{(L)}(\mathbf{q}_i) >_{m^*} |^2$$

$$| < \Psi_i^{(L)}(\mathbf{q}_i)|e^{i\mathbf{k}\cdot\mathbf{R}_j}|\Psi_f^{(L)}(\mathbf{q}_i) >_m |^2\delta(I_K + \hbar^2|\mathbf{k}|^2/2m_e + E_f^{(L)} - E_i^{(L)}) \tag{2.17}$$

It is convenient to introduce a function that keeps track of the probability that an energy transfer ϵ occurs, given a recoil momentum $\mathbf{k}$. Such a function may be conveniently defined through

$$p_{j,\mathbf{k}}(\epsilon) = \sum_f | < \Psi_i^{(L)}(\mathbf{q}_i)|e^{-i\hat{S}_D}|\Psi_f^{(L)}(\mathbf{q}_i) >_{m^*} |^2| < \Psi_i^{(L)}(\mathbf{q}_i)|e^{i\mathbf{k}\cdot\mathbf{R}_j}|\Psi_f^{(L)}(\mathbf{q}_i) >_m |^2\delta(\epsilon + E_f^{(L)} - E_i^{(L)}) \tag{2.18}$$

This function may be used to develop a perhaps more intuitive version of the decay rate, given by

$$\Gamma_j = \sum_{\mathbf{k}}\int p_{j,\mathbf{k}}(\epsilon)\Gamma_{j,\mathbf{k}}(\epsilon)d\epsilon \tag{2.19}$$

with

$$\Gamma_{j,\mathbf{k}}(\epsilon) = \frac{2\pi}{\hbar}|V(\mathbf{k})|^2\delta(I_K + \hbar^2|\mathbf{k}|^2/2m_e - \epsilon) \tag{2.20}$$

These formulas suggest a point of view in which there exists a probability p of transferring an energy ϵ from the lattice, and that energy transfer drives a reaction with a partial rate that may be computed essentially without consideration of lattice effects.

The computation of $p_{j,\mathbf{k}}(\epsilon)$ is of course in general quite complicated. As defined, this function is proportional to a lineshape function that might be associated with a process that has an associated recoil and that modifies the underlying phonon mode structure. The recoil term by itself is generally computed by evaluating contributions from 0,1,...,n-phonon pieces; the mode-matching physics is usually treated in perturbation theory. In the case of a thermal lattice, this function would result in a rather standard few-meV wide line that is perhaps shifted by a few-meV. However, if there exist highly excited phonon modes that jump a band gap as a result of modifications to the lattice due to recoil, then the function must shift in energy by an amount $n\delta\omega$ for each mode that jumps, as would a line profile under corresponding circumstances.

In general, there will be a probability that sufficient recoil will occur to cause a gap jumps, as well as a probability that the recoil is insufficient to cause gap jumps. In this case, the function $p_{j,\mathbf{k}}(\epsilon)$ will have two pieces – one that gives energy transfer, and one that does not. Of course, if no energy transfer occurs due to gap-jumping, then the energy transfer from the lattice from thermal recoil effects alone will be too small to drive any of the reactions that we consider below.

Consequently, our interest is focussed only on the part of $p_{j,k}(\epsilon)$ that corresponds to situations where gap-jumping occurs. Mathematically, the probability $p_{j,k}(\epsilon)$ will be of the form

$$p(\epsilon) = |T|^2 p_{jump}(\epsilon - \sum n\hbar\delta\omega) + (1 - |T|^2)p_{no\ jump}(\epsilon) \tag{2.21}$$

where $|T|^2$ is the probability that the recoil was sufficient to cause a jump, and where $p_{jump}(\epsilon)$ and $p_{no\ jump}(\epsilon)$ are complicated functions of energy whose precise shapes will be of little concern to us, as long as $p_{jump}(\epsilon)$ is narrow compared to the energy transfer $\sum n\hbar\delta\omega$. In what follows, we will discuss this further. Given that $p_{no\ jump}(\epsilon)$ is of no interest in computing reaction rates for anomalous processes, we will neglect it henceforth.

We have computed previously the line shape for lattice energy transfer as a function of ϵ in the case of neutron capture,[12] under conditions where there was no direct recoil (in this case, the energy transfer occurs through a mass change rather than through the creation of a vacancy). We found that the probability for energy transfer in the case of a single gap-jumping phonon mode initially in a number state was a shifted Gaussian

$$\sum_f | < \Psi_i^{(L)}(\mathbf{q}_i)|e^{-i\hat{S}_D}|\Psi_f^{(L)}(\mathbf{q}_i) >_{m^*} |^2 \sim e^{-\beta(\epsilon - n<\hbar\delta\omega>)^2} \tag{2.22}$$

where ϵ is the actual energy transfer from the lattice, and $n < \hbar\delta\omega >$ is the expectation value of the energy transfer. The line is narrow; $\beta^{-1} \sim n < (\hbar\delta\omega)^2 >$. The spread is due to the range of frequencies of the final state modes into which a single gap-jumping mode projects.

Perhaps more relevant (since it is not clear how to excite a phonon mode to a number state) is the probability distribution in the case of a highly excited gap-jumping continuum phonon that is initially in a classical state. A classical state $|\alpha >$ can be constructed from number states, and it is well known that a Poisson distribution is produced:[18]

$$|\alpha >= e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |n > \tag{2.23}$$

which leads to

$$| < n|\alpha > |^2 = e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!} \tag{2.24}$$

A highly excited classical state is well approximated by a shifted Gaussian around the mean number of phonons $< n >= \alpha^2$, and with a variance $< \Delta n^2 >=< (n - < n >)^2 >=< n >$. For an energy transfer of 1 MeV, on the order of 10^8 or more phonons must be present, which implies a narrow probability distribution $\sqrt{< \Delta n^2 >}/ < n > \sim 10^{-4}$. Consequently, both for number states and for classical states, it will be an excellent approximation to take

$$p(\epsilon) \approx \delta(\epsilon - \sum_{m^*} < n_{m^*} >< \hbar\delta\omega_{m^*} >) \tag{2.25}$$

Here we must extend our analysis to include recoil effects in the probability function. In the case of electron ejection the recoil is relatively weak, and the essential effect that occurs is that the transfer of energy is prevented unless the recoil energy is sufficiently strong to permanently dislodge the nucleus.

For most of the values of the lattice energy transfer ϵ that are of potential interest, the recoil momentum is sufficiently great that a vacancy is created with certainty. An accurate calculation of the recoil matrix element requires a model for inter-nuclear potentials in the lattice, and is beyond the scope of this work. In essence, a nucleus that recoils must overcome a potential barrier to land in a new and inequivalent site in order to satisfy the requirement that the phonon modes be irreversibly changed. We assume that the energy of the vacancy plus displaced nucleus lies at an energy E_d relative to the initial configuration, that the barrier energy is E_b, and that the potential barrier is adequately modeled by a parabola over a distance d

$$V_b(x) = E_b - \frac{1}{2}\alpha x^2 \tag{2.26}$$

with $V_b(\pm d/2) = E_d$. We then obtain an estimate of the efficiency for tunneling for $E_d < E_r < E_b$ to be

$$\sum_f | < \Psi_i^{(L)}(\mathbf{q}_i)|e^{i\mathbf{k}\cdot\mathbf{R}_j}|\Psi_f^{(L)}(\mathbf{q}_i) >_m |^2 = |T(\mathbf{k})|^2 \approx \exp\left\{-\frac{\pi}{2}\frac{(E_b - E_r)}{\sqrt{(E_b - E_d)(\hbar^2/2Md^2)}}\right\} \tag{2.27}$$

where E_r is the recoil energy of the Pd nucleus $\hbar^2|\mathbf{k}|^2/2M$. For $E_r < E_d$, a vacancy is not created, and we take $T = 0$; for $E > E_b$ we assume that the decay occurs freely, and $|T|^2 = 1$.

We have found that the frequency-shift of gap-jumping phonon modes leads ultimately to the appearance of an isolated system reaction rate evaluated at an anomalous energy transfer ϵ; the recoil effects primarily cuts off the reaction rate at low energy. Precisely where this cut-off occurs as a function of lattice energy transfer depends strongly on the details of the chemical environment in the vicinity of the nucleus, details that are not easily available at present. The parabolic tunneling model presented here allows us to obtain predictions given "reasonable" estimates of the excitation energies and barriers.

These approximations lead to an estimate of the reaction rate per nucleus given by

$$\Gamma_j = \Gamma_0(\Delta E_L)\ |T(\mathbf{k})|^2 \tag{2.28}$$

where the lattice energy transfer is

$$\Delta E_L = \sum_{m^*} < n_{m^*} >< \hbar\delta\omega_{m^*} > \tag{2.29}$$

and where the rate $\Gamma_0(\epsilon)$ is obtained by summing over $\mathbf{k}$ to yield

$$\Gamma_0(\epsilon) = \frac{2\pi}{\hbar}|V(\mathbf{k})|^2\rho(E_f) \tag{2.30}$$

where $\mathbf{k}$ is evaluated at $\hbar^2|\mathbf{k}|^2/2m_e = \epsilon - I_K$. Inserting expressions for $V(\mathbf{k})$ and for $\rho(E_f)$, we obtain

$$\Gamma_0(\epsilon) = \frac{24N_{1s}}{\pi Z}\frac{I_H}{\hbar}\left[\frac{\epsilon}{I_H}\right]^{\frac{1}{2}}\frac{1}{[1+(\epsilon/Z^2I_H)]^2} \tag{2.31}$$

where I_H is 13.6058 eV.

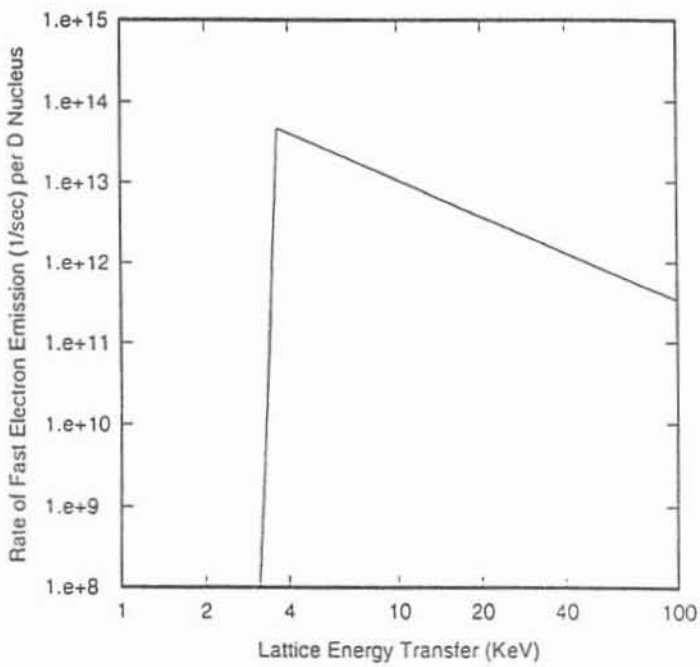

Figure 2: Predicted fast electron emission rate from deuterons as a function of lattice energy transfer.

Results for K-shell ejection from deuterium and from Pd in PdD are shown in Figures 2 and 3. The threshold for emission of fast electrons occurs when the recoil energy of the nucleus becomes equal to the barrier energy for vacancy creation; this occurs in the nonrelativistic limit at

$$\Delta E = 1835\ A\ E_d \tag{2.32}$$

In the case of Pd vacancy production, we have used $E_d = 6eV$ and $E_b = 10eV$ as our "reasonable" estimates of energies required to irreversibly create a vacancy. In the case of deuterium, we have selected the parameters $E_{=}0.7eV$, $E_b = 1.0eV$ and $d = 1a_0$; while the excitation to nearby octohedral or tetrahedral sites will occur with energies below 0.3eV, 1 eV should be sufficient to move the deuterium to a more remote local. Relativistic formulas have been used to estimate the recoil energy in the Figures.

It should be noted that the phonon modes that jump a band gap are different for these two processes. We have discussed gap-jumping in the case of Pd vacancy creation above; this process should occur with strong excitation of the lowest optical phonon modes. In the case of deuterium vacancy creation, we rely on a postulated set of isolated vacancy impurity modes that correspond to cells with different numbers of deuterons in the vicinity of a host metal vacancy.

The decay rates per nucleus for these processes are seen to be very large, consequently the total lattice decay rates will be so great that it must be questioned under what conditions the model will be valid. We will examine this question in the following section.

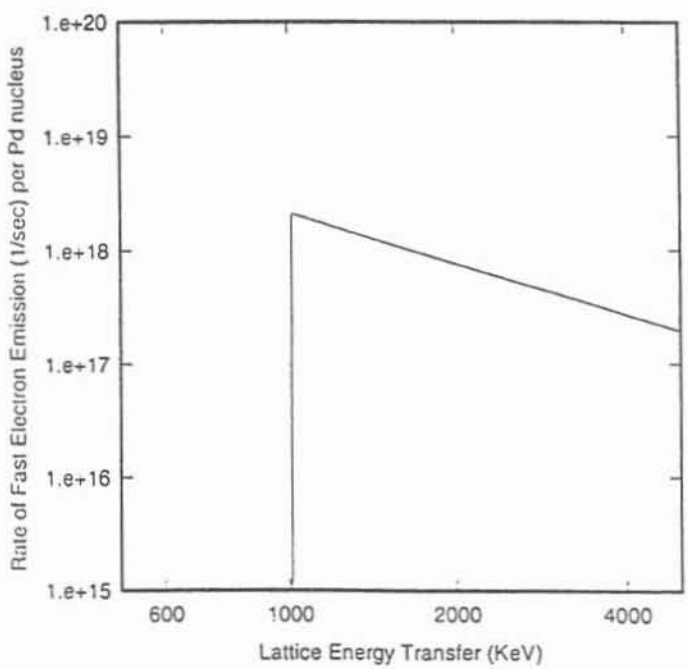

Figure 3: Predicted fast electron emission rate from Pd nuclei as a function of lattice energy transfer.

3. Coupled Reactions

The reaction rate estimates presented in the last section indicates that a lattice with very highly excited gap-jumping phonon modes will decay by fast electron emission very rapidly. The characteristic decay rates can be greater than 10^{10} sec^{-1} per nucleus, which if correct, would perhaps imply a total lattice decay rate between 10^{25} and 10^{30} sec^{-1} for the total volume over which the phonon modes extend; these total rates are much too fast to be physical.

Towards the resolution of this problem, there are a number of issues that must be considered. For example, if the lattice decay rate is so fast, then it becomes problematic how the lattice could have been so highly excited originally. In the process of exciting the gap-jumping modes, a fast decay should have occured once sufficient excitation was present to enable Coulomb decay to occur at all at much slower rates. Under these conditions, the theory described in Section II would apply, and no inconsistencies would be present.

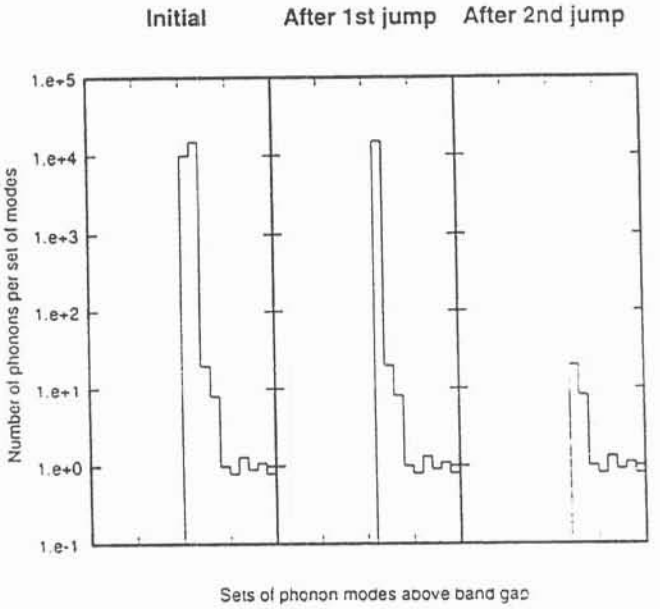

Figure 4: Pictorial of phonon mode excitation near the band gap before and after gap-jumping.

The situation becomes very much more interesting under conditions where the initial moderately-excited modes jump the gap to reveal new gap-jumping modes that are much more highly excited. When downward gap-jumping occurs, it is the lowest phonon modes above the gap that actually jump (see Figure 4). If several jumps occur in succession, it is always the lowest modes that jump in any specific reaction; consequently, phonon modes are stripped away from the bottom in sequence, much like the peeling of an onion.

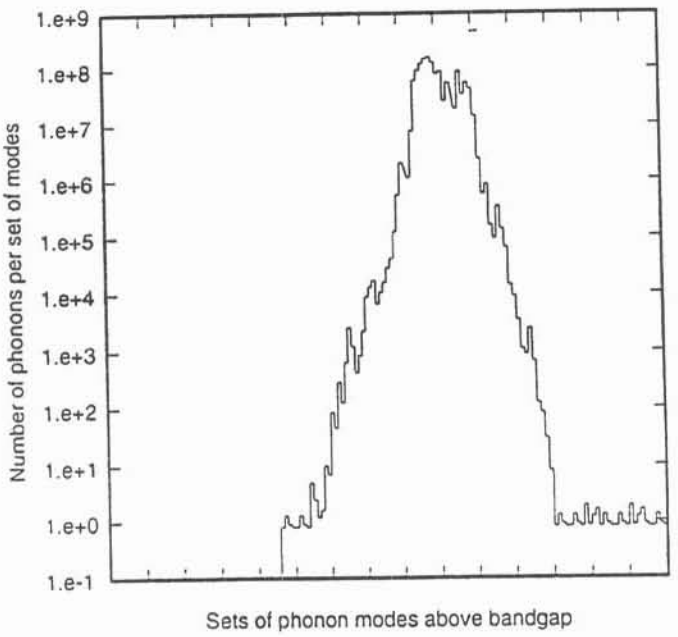

Figure 5: Pictorial of high phonon mode excitation that is shielded from the band gap by modes with low excitation.

Under such conditions, it can no longer be argued that the phonon population could not have built up without provoking a fast Coulomb decay; highly excited modes that are shielded from the gap by unexcited modes are free to build up to very high levels, as illustrated in Figure 5. Nevertheless, we would be certain that if the resulting rate estimate when these modes did finally jump, were on the order of 10^{25} to 10^{30} $\sec^{-1}$, that rate estimate must be in error.

The resolution to this problem is that the two reactions would become coupled together in the Raman sense, and reaction rates must be computed using a theory which fundamentally treats the processes as coupled. The mechanisms that would produce very high phonon populations would however likely not result in such high selectivity as to produce just one or two reactions, rather it is more likely that 10^5 to 10^8 phonon modes would cause reactions at a time. Consequently, we require a theory for bursts of large numbers of reactions.

The starting point for our discussion is the expression for a single isolated event from the last section, recast as

$$\Gamma_j = \frac{2\pi}{\hbar} \sum_{\mathrm{k}} |V(\mathrm{k})|^2 \int d\epsilon \; p_{j,\mathrm{k}}(\epsilon) \delta(I_K + \hbar^2 |\mathrm{k}|^2 / 2m_e - \epsilon) \tag{3.1}$$

Taking the probability function to be sharply peaked in energy, we obtain

$$\Gamma_j = \frac{2\pi}{\hbar}\sum_{\mathbf{k}}|V(\mathbf{k})|^2|T(\mathbf{k})|^2\delta(I_K+\hbar^2|\mathbf{k}|^2/2m_e- < n >< \delta\hbar\omega >) \tag{3.2}$$

We have adopted the notation $< n >< \delta\hbar\omega >$ for $\sum_{m^*} < n_{m^*} >< \delta\hbar\omega_{m^*} >$. This form is most convenient for generalization.

In the case of two coupled reactions, we obtain

$$\Gamma_{j_1,j_2} =$$

$$\frac{\pi}{\hbar}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2}\left|\frac{V(\mathbf{k}_1)V(\mathbf{k}_2)T(\mathbf{k}_1)T(\mathbf{k}_2)}{I_K+\hbar^2|\mathbf{k}_1|^2/2M- < n_1 >< \delta\hbar\omega_1 > -i\hbar\gamma}+\frac{V(\mathbf{k}_2)V(\mathbf{k}_1)T(\mathbf{k}_2)T(\mathbf{k}_1)}{I_K+\hbar^2|\mathbf{k}_2|^2/2M- < n_1 >< \delta\hbar\omega_1 > -i\hbar\gamma}\right|^2$$

$$\delta(2I_K+\hbar^2|\mathbf{k}_1|^2/2m_e+\hbar^2|\mathbf{k}_2|^2/2m_e- < n_1 >< \delta\hbar\omega_1 > - < n_2 >< \delta\hbar\omega_2 >) \tag{3.3}$$

The interaction matrix element is now composed of two terms, as is appropriate for a second order process. The relative phases between the various matrix elements will generally be random; when averaged over all pairs of sites in the lattice, the interference terms will not contribute due to cancellation. Consequently, it is of interest to focus on a site-averaged version of the decay rate

$$\overline{\Gamma}_{j_1,j_2} = \frac{2\pi}{\hbar}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2}\frac{|V(\mathbf{k}_1)V(\mathbf{k}_2)T(\mathbf{k}_1)T(\mathbf{k}_2)|^2}{(I_K+\hbar^2|\mathbf{k}_1|^2/2M- < n_1 >< \delta\hbar\omega_1 >)^2+\hbar^2\gamma^2}$$

$$\delta(2I_K+\hbar^2|\mathbf{k}_1|^2/2m_e+\hbar^2|\mathbf{k}_2|^2/2m_e- < n_1 >< \delta\hbar\omega_1 > - < n_2 >< \delta\hbar\omega_2 >) \tag{3.4}$$

To obtain the total decay rate, this formula must be summed over all pairs of nuclei in a domain in which the highly excited phonon modes exist.

Further generalization to larger numbers of coupled reactions is straightforward; we obtain

$$\overline{\Gamma}_N = \frac{2\pi}{\hbar}\sum_{\mathbf{k}_1}\cdots\sum_{\mathbf{k}_N}\frac{|V(\mathbf{k}_1)T(\mathbf{k}_1)|^2\cdots|V(\mathbf{k}_N)T(\mathbf{k}_N)|^2}{\prod_j^{N-1}\left[(jI_K+\sum_i^j\hbar^2|\mathbf{k}_i|^2/2M-\sum_i^j < n_i >< \delta\hbar\omega_i >)^2+\hbar^2\gamma^2\right]}$$

$$\delta(NI_K+\sum_j^N\hbar^2|\mathbf{k}_j|^2/2m_e-\sum_j^N < n_j >< \delta\hbar\omega_j >) \tag{3.5}$$

This formula, summed over all sets of N nuclei in the domain of the highly excited phonon modes, would give the decay rate for an N-particle "burst".

The appearance of such high order matrix elements in the calculation of reaction rates is rare in the literature. A currently active area of research wherein high order matrix elements are calculated routinely is the area of laser-induced multi-photon ionization.[19] A number of methods have proven to be successful in these calculations, including Floquet theory coupled with R-matrix methods,[20]

and time-dependent Hartree-Fock theory.[21] These types of methods could be used in the present case with some modifications.

It is possible that reliable rates for the present problem could be obtained using a method of steepest descents. The basic idea is as follows: The largest total decay rates would be obtained in the limit that all of the individual steps were resonant; however, many of the transitions will likely take place off of resonance if an adequate degree of phonon excitation is not present – this would be especially true of the earliest decays, which were postulated above to be at best marginal. As a result, excitation energy must be borrowed from those phonon modes that are well above threshold in order for decays to occur with sufficient recoil to cause phonon modes to jump the gap in cases where the phonon excitation is marginal.

Consequently, it should be possible to select an optimum set of decay energies $\{|\mathrm{k}|^2\}$, subject to the constraint that overall energy conservation be maintained, that would give the largest possible value for the product inside the summation of equation (3.5). This optimum would likely have many decays occuring on resonance, with as few decays as possible loaning energy to those decays that are marginal or forbidden. Away from this optimum selection of decay energies, there would be less contribution to the summations; the reduction in the contribution would by definition be second order away from the optimum, and this could be evaluated algebraically using Gaussian integrations.

These arguments imply the following approximation scheme. Define the variational function

$$I[\mathrm{k}_1 \cdots \mathrm{k}_N] = \frac{|V(\mathrm{k}_1)T(\mathrm{k}_1)|^2 \cdots |V(\mathrm{k}_N)T(\mathrm{k}_N)|^2}{\prod_j^{N-1}\left[(jI_K + \sum_i^j \hbar^2|\mathrm{k}_i|^2/2M - \sum_i^j < n_i >< \delta\hbar\omega_i >)^2 + \hbar^2\gamma^2\right]}$$
$$-\lambda(NI_K + \sum_j^N \hbar^2|\mathrm{k}_j|^2/2m_e - \sum_j^N < n_j >< \delta\hbar\omega_j >) \qquad (3.6)$$

where λ is a Lagrange multiplier. Compute the optimum distribution of decay energies through

$$\frac{\partial}{\partial k_i} I[\mathrm{k}_1 \cdots \mathrm{k}_N]\Big|_{\{\mathrm{k}\}_0} = 0 \qquad (3.7)$$

Next, develop a Gaussian model around the optimum set of decay energies

$$J(\mathrm{k}_1 \cdots \mathrm{k}_{N-1}) = J_0 e^{-(\mathrm{k}-\mathrm{k}_0)^T \cdot \mathrm{G} \cdot (\mathrm{k}-\mathrm{k}_0)} \qquad (3.8)$$

where we have adopted a notation k for a very large vector composed of all individual components for $\mathrm{k}_1 \cdots \mathrm{k}_{N-1}$; the optimum for the momenuta is now denoted by k_0. The partial sum $J(\mathrm{k}_1 \cdots \mathrm{k}_{N-1})$ is defined by

$$J(\mathbf{k}_1 \cdots \mathbf{k}_{N-1}) = \sum_{\mathbf{k}_N} \frac{|V(\mathbf{k}_1)T(\mathbf{k}_1)|^2 \cdots |V(\mathbf{k}_N)T(\mathbf{k}_N)|^2}{\prod_j^{N-1} \left[(jI_K + \sum_i^j \hbar^2 |\mathbf{k}_i|^2/2M - \sum_i^j < n_i >< \delta\hbar\omega_i >)^2 + \hbar^2\gamma^2 \right]}$$

$$\delta(NI_K + \sum_j^N \hbar^2 |\mathbf{k}_j|^2/2m_e - \sum_j^N < n_j >< \delta\hbar\omega_j >) \tag{3.9}$$

The matrix G is obtained by matching second derivatives around the optimum. Finally, the total decay rate is computed using

$$\overline{\Gamma}_N = \frac{2\pi}{\hbar} \sum_{\mathbf{k}_1} \cdots \sum_{\mathbf{k}_{N-1}} J_0 e^{-(\mathbf{k}-\mathbf{k}_0)^T \cdot \mathbf{G} \cdot (\mathbf{k}-\mathbf{k}_0)} \tag{3.10}$$

taking advantage of algebraic Gaussian integration formulas.

We have not carried out any computations for the rates of "bursts" yet with this model; this project is left for future work. There is little question that the excitation of many low-lying modes will result in decays that occur through bursts, and in principle we will be able to estimate rates for the bursts, either with the formulas presented above or through other routes. It is of interest to inquire as to what distribution of decay products would be expected within a burst, assuming that more than one possible decay channel occurs. The theory for bursts presented above is readily generalized in the case of multiple decay channels, with little change in essential physics. The distribution of decay products would be determined in principle by performing sets of burst rate calculations with slightly different sets of decay channels around whatever set of decay channels maximizes the total burst rate.

As these models have not yet been studied, we cannot say at this point with certainty what distribution of decay products should be expected in general. Nevertheless, the appearance of each individual decay process occurs in the total burst rate formula through terms that are very much like those that occur in the single-event version of Fermi's Golden Rule rate. One might postulate that the burst rate fraction f_j for a single decay channel could be estimated by computing the ratio of the single-event rate with the total of all possible single-event rates for all available decay channels dependent on the same phonon modes

$$f_j = \frac{\Gamma_j}{\sum_i \Gamma_i} \tag{3.11}$$

Such a formula might be useful in a "low rate" limit, corresponding to the I^n dependence observed for n-photon absorption in the low intensity regime. Whereas the muiti-photon rates saturate at high I, a non-perturbative treatment of the bursts would likely show "saturation effects". In this limit, a weak channel competing with a stronger channel would have a lower fraction f_j, but it

is not clear at this point by how much. In the sections that follow, lacking more precise tools to quantify reaction rates, we will continue to calculate Fermi's Golden Rule rates for the various channels as single events, keeping in mind that these estimates are only qualitative indicators of actual rates and fractions.

4. Deuteron Acceleration and Neutron Production

Another dominant decay mechanism for a lattice that possesses very highly excited gap-jumping phonon modes is Coulomb-induced nucleus-nucleus recoil. For example, if two Pd nuclei in PdD recoil off of each other with 50 eV energy input from the lattice, at least two Pd vacancies will be created; depending on the details of the outcome, this process could self-consistently lead to energy transfer from the lattice caused by highly excited optical phonon mode jumping a band gap to increase the number of "vacancy" optical phonon models.

Perhaps the most interesting example of this process is lattice decay by deuteron recoil off of other nuclei, for the reason that fast deuterons produced in this way could in principle fuse with other deuterons in the lattice resulting in *dd*-fusion neutrons at 2.45 MeV. We have estimated decay rates for deuteron-deuteron recoil as a function of lattice energy, and used these rates to estimate neutron production rates; the results are quite interesting, and are not inconsistent with some of the experimental claims for the production of neutrons.

Fermi's Golden Rule applied to lattice-induced deuteron-deuteron recoil gives rise to the following rate estimate

$$\Gamma = \frac{2\pi}{\hbar} \sum_f \sum_{\mathbf{K}} | < \Psi_i | \hat{V} | \Psi_f > |^2 \delta(2I_D + \hbar^2 |\mathbf{K}|^2 / 2\mu + E_f^{(L)} - E_i^{(L)}) \tag{4.1}$$

where I_D is the binding energy of a deuteron, $\hbar^2|\mathbf{K}|^2/2\mu$ is the relative kinetic energy of the two deuterons that have recoiled away from each other, and the potential $\hat{V}$ is the Coulomb interaction

$$\hat{V} = \sum_{j<j'} \frac{e^2}{|\hat{\mathbf{R}}_j - \hat{\mathbf{R}}_{j'}|} \tag{4.2}$$

The arguments of Section II can be used here when the energy transfer from the lattice is dominated by the frequency shift of highly excited gap-jumping phonon modes. We focus on the matrix element in the case of the recoil of two specific neighboring deuterons, in which case the Coulomb matrix element can be written in terms of phonon amplitudes

$$< \Psi_i | \hat{V}_{j,j'} | \Psi_f > = < \Psi_i(\mathbf{q}_i) | \hat{V}_{j,j'} e^{-i\hat{S}_D} | \Psi_f(\mathbf{q}_i) > \tag{4.3}$$

where the Duschinsky operator takes into account modifications in the phonon mode structure. As before, the matrix element separates approximately into a piece responsible for the primary energy transfer, and a piece containing the majority of non-gap-jumping phonon modes that are involved in the recoil process

$$< \Psi_i(\mathbf{q}_i)|\hat{V}_{j,j'}e^{-i\hat{S}_D}|\Psi_f(\mathbf{q}_i) > \approx < \Psi_i(\mathbf{q}_i)|e^{-i\hat{S}_D}|\Psi_f(\mathbf{q}_i) >_{m^*} < \Psi_i(\mathbf{q}_i)|\hat{V}_{j,j'}|\Psi_f(\mathbf{q}_i) >_m \qquad (4.4)$$

The initial and final states $\Psi_i(\mathbf{q}_i)$ and $\Psi_f(\mathbf{q}_i)$ have the same energy, and total energy is conserved in this type of recoil reaction. Following the arguments of the last two sections, the Duschinsky matrix element will be sharply peaked around an energy transfer of $< n >< \hbar\delta\omega >$ for the m^* phonon modes that jump the gap. Because of energy conservation, this energy becomes available for the local Coulomb repulsion between two nuclei. We obtain

$$\Gamma_{j,j'} = \frac{2\pi}{\hbar}\sum_f\sum_{\mathbf{K}} | < \Psi_i(\mathbf{q}_i)|e^{-i\hat{S}_D}|\Psi_f(\mathbf{q}_i) >_{m^*} |^2 | < \Psi_i(\mathbf{q}_i)|\hat{V}_{j,j'}|\Psi_f(\mathbf{q}_i) >_m |^2$$
$$\delta(2I_D + \hbar^2|\mathbf{K}|^2/2\mu + E_f^{(L)} - E_i^{(L)}) \qquad (4.5)$$

which evaluates approximately to

$$\Gamma_{j,j'} = \frac{2\pi}{\hbar}\sum_f\sum_{\mathbf{K}} | < \Psi_i(\mathbf{q}_i)|\hat{V}_{j,j'}|\Psi_f(\mathbf{q}_i) >_m |^2 \delta(2I_D + \hbar^2|\mathbf{K}|^2/2\mu - < n >< \hbar\delta\omega >) \qquad (4.6)$$

This formula assumes that the recoil is sufficiently great to insure that deuterons are truly irreversibly removed from their cells so that the m^* phonon modes jump a bandgap. Our neglect of the tunneling factor in this formula will mean that our results will be valid only for an energy transfer exceeding 2-3 eV.

The local Coulomb repulsion matrix element is strongly dependent on the local chemical environment, since a large recoil can only occur when the deuterons are close together. Focusing on the interesting case of large momentum transfer, we have approximated the relative probability amplitudes of deuterons in the lattice using the molecular D_2 ground state wavefunction:

$$< \Psi_i(\mathbf{q}_i)|\hat{V}_{j,j'}|\Psi_f(\mathbf{q}_i) >_m \approx < \Psi_{D_2}(\mathbf{r})|\frac{e^2}{|\mathbf{r}|}|\Psi_{\mathbf{K}}(\mathbf{r}) > \qquad (4.7)$$

In this formula. the final state $\Psi_{\mathbf{K}}(\mathbf{r})$ represents a dissociated molecule with a relative momentum between the deuterons of $\hbar\mathbf{K}$. This type of approximation has been used by many authors to provide molecular estimates of *dd*-fusion rates thought to be relevant to the problem of fusion rates in PdD. While the applicability of this type of model in the case of fusion reactions may be

questionable, it is very likely a much better approximation in the case of recoil, since the recoil matrix element samples phase space at larger inter-deuteron separations; the recoil matrix elements appear to be far less sensitive to variations in the potential.

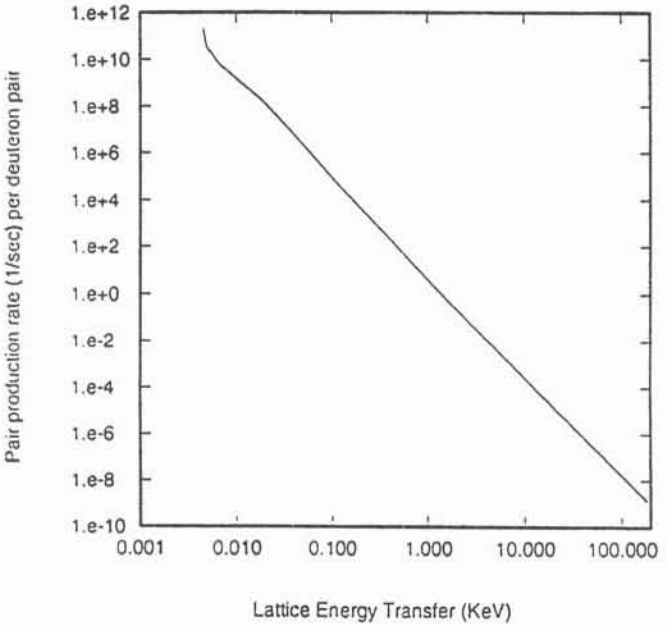

Figure 6: Decay rate per deuteron pair for lattice-induced Coulomb recoil.

It was convenient for us to evaulate the reaction rate using a coupled-channel model, which is an improvement over the approximations discussed above. In this model, the unperturbed ground state radial wavefunction was computed by solution of the unperturbed radial Schrodinger equation

$$EP_o(r) = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}P_o(r) + V(r)P_o(r) \tag{4.8}$$

using the parameterization[22]

$$V(r) = e^{-\alpha r}\left[\frac{e^2}{r} - b\right] \tag{4.9}$$

with $\alpha = 0.886/a_0$ and $b = 2.630 I_H$. The continuum channel was computed using

$$\frac{\hbar^2|\mathbf{K}|^2}{2\mu}P(r) = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}P(r) + V(r)P(r) + \frac{e^2}{r}P_o(r) \tag{4.10}$$

subject to the boundary condition

$$P(r) \longrightarrow f(\mathbf{K})e^{i|\mathbf{K}|r} \tag{4.11}$$

The decay rate is obtained by integrating the outward flux over a sphere at large r; this results in

$$\Gamma_{j,j'} = \frac{\hbar|\mathbf{K}|}{\mu}|f(\mathbf{K})|^2 \tag{4.12}$$

The results of this calculation are shown in Figure 6.

Predicted by this theory are fast deuterons that can in principle fuse with neighboring deuterons. Taking the results of the deuteron-deuteron recoil calculation discussed above, we combined the production rate of fast deuterons with the neutron yield (including the energy loss of the deuterons on the host palladium nuclei) to produce an estimate of the *dd*-fusion neutron rate. The results are shown in Figure 7. Keeping in mind the discussion of Section 3, this process will compete with fast electron production at lattice transfer energies above a few kilovolts, which will have the ultimate effect of essentially eliminating this channel. In metal hydrides with deeper deuteron potentials (such as TiD_2), this competition will be put off to higher lattice transfer energy, resulting in larger neutron production rates.

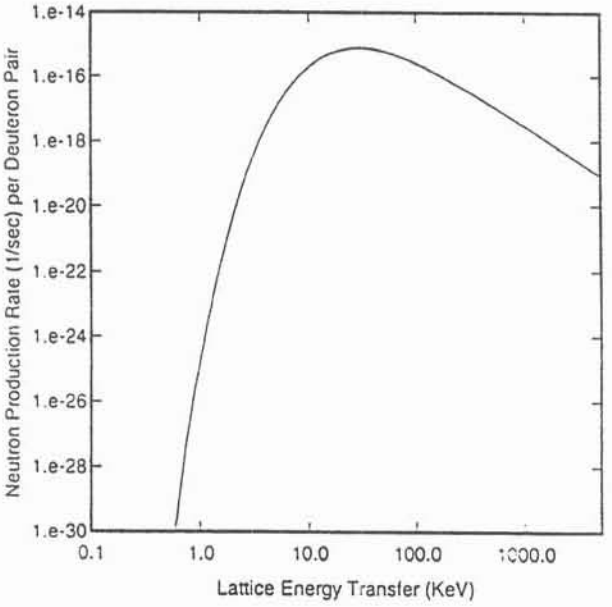

Figure 7: Production rate of *dd*-fusion neutrons through deuteron-deuteron recoil followed by fusion.

For completeness, we estimated reaction rates for the rare process in which the Coulomb exchange causes the two initial recoiling deuterons to fuse with each other. The resulting rate is observed to increase by about thirty orders of magnitude over the ground state D_2 fusion rate, but in our calculations did not compete with the deuteron-other-deuteron fusion rate given above.

5. Lattice-induced Bēta Decays

We have thus far discussed the decay of a highly excited lattice through atomic decay channels. The lattice may also decay through available nuclear channels, subject to the constraints discussed above, and in competition with other open channels such as electron recoil. In this section, we examine lattice-induced reactions mediated by the weak force.

The basic theory for lattice-induced electron capture reactions and beta decays follows immediately from the theory outlined in Sections 2 and 3. The Fermi's Golden Rule estimate for a lattice-induced decay is

$$\Gamma = |T(\mathbf{k})|^2 \Gamma_0(\Delta E_L) \tag{5.1}$$

where $|T|^2$ is the probability that the recoil is sufficient to irreversibly create a vacancy, and where $\Gamma_0(\Delta E_L)$ is the rate computed assuming that an energy ΔE_L is transferred from the lattice. We have computed lattice-induced decay rates according to this estimate based on the $f\tau$ theory discussed in Ref. 23.

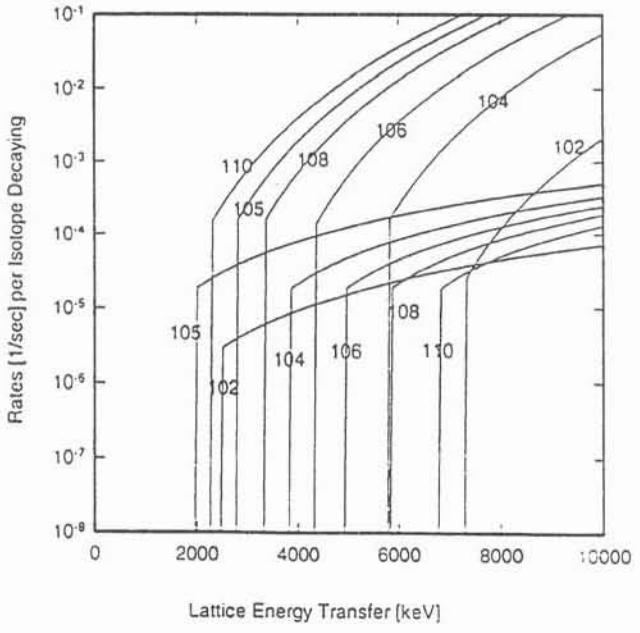

Figure 8: Lattice-induced electron capture and beta decay rates for the Pd nuclei. Curves that continue to rise are e^- decay; curves that are lower are electron capture.

As a function of lattice energy transfer, the first decay to occur is electron capture from ^{105}Pd to ^{105}Rh. This may be interesting, in that the first two excited states of ^{105}Rh occur at 129.6 KeV

and at 149.1 KeV; emission at these energies is claimed to have been observed in glow discharge experiments at Luch. Gamma lines produced by the decay of ^{105}Rh back to ^{105}Pd have also been claimed in these experiments.[7] In Figure 8 is shown estimates of the lattice-induced electron capture rates and beta decay rates for the stable Pd nuclei.

Isotopes that are already unstable against beta decay can decay more rapidly with extra energy input from the lattice. We studied the enhancement of the beta decay of ^{107}Pd to ^{107}Ag through this mechanism. As expected, no enhancement occurs until the recoil becomes sufficiently great to cause a vacancy to be formed. With the model of Section 2, this does not occur until about 950 KeV. At this energy, one would expect to observed characteristic gamma emission from excited ^{107}Ag at 93 KeV.

Tritium decay can be enhanced through this type of mechanism, and lattice-induced electron capture on ^{3}He can in principle produce tritium, although precisely which vacancy impurity bands ^{3}He decay would involve is not clear at this point. The rates for these processes are shown in Figure 9.

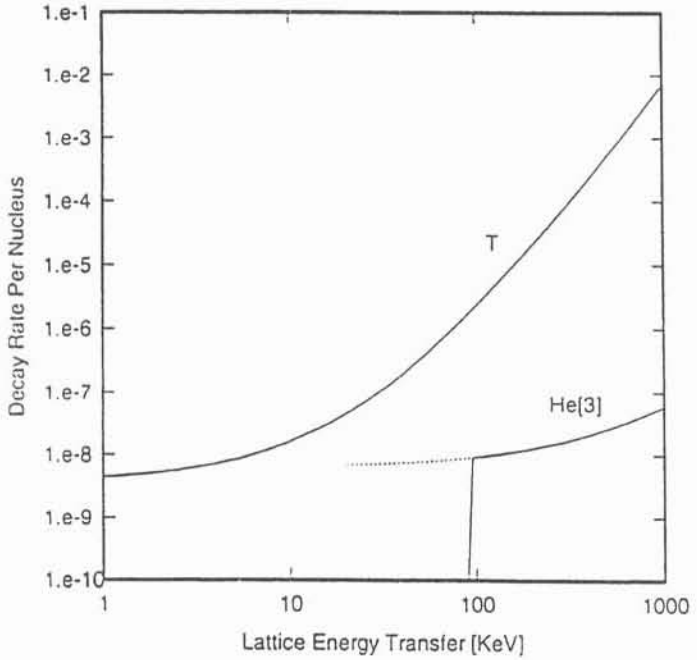

Figure 9: Lattice-enhanced tritium beta decay; lattice-induced ^{3}He electron capture to make tritium.

6. Lattice-Induced Alpha Decay

If the energy transfer is sufficiently great, alpha decay becomes an available decay channel. The analysis of lattice-induced alpha decay is particularly simple, in that the decay always provides sufficient recoil for local vacancy formation. We have calculated the rate for lattice-induced alpha decay of Pd nuclei; the results are shown in Figure 10. The first isotope to decay as a function of energy is ^{102}Pd; energy transfers in excess of about 5 MeV are required for this process.

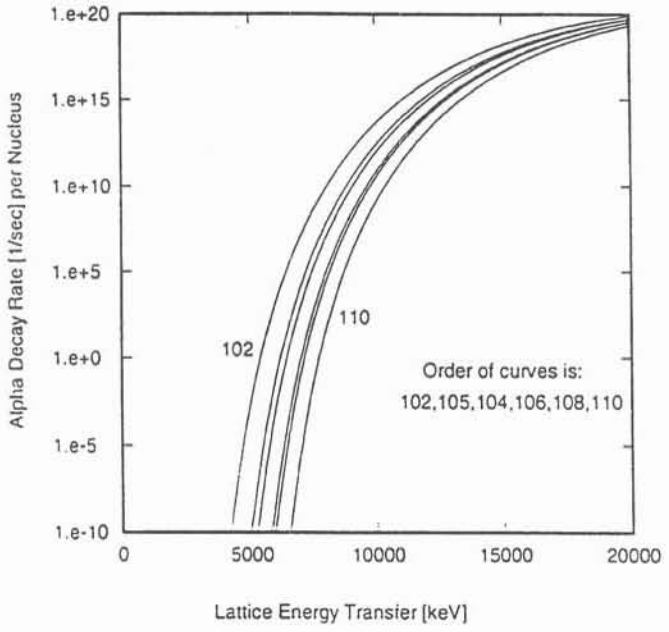

Figure 10: Lattice-induced alpha decay of the Pd isotopes.

Larger energy transfers can lead to more complicated decay channels; for example, proton and neutron decays turn on near 10 MeV lattice energy transfer. We have examined reaction rates for a wide variety of fission decay channels; these will be discussed further elswhere. Qualitatively, the rates for these decays go something like those for alpha decay, but require significantly more energy; from 20 MeV to more than 50 MeV of energy transfer will lead to a wide range of open lattice-induced fission channels. At such large energy transfer where alpha and fission decay processes are allowed, these reactions are predicted to be the dominate decay channels.

7. Discussion and Conclusions

We have presented a new theory for lattice-induced reactions, which a predicted to be driven by highly excited gap-jumping phonon modes. The reaction mechanisms discussed in this work were motivated by the many recent claimes of observations of anomalies in PdD, in other metal deuterides, and in metal hydrides.

At low energy transfer, the dominant lattice decay mechanisms are the Coulomb-mediated nucleus-nucleus recoils; in the case of deuteron-deuteron recoils, *dd*-fusion at low levels is predicted. The reaction rates computed for this process are of the correct order of magnitude to be consistent with the claimed experimental neutron emission, at low lattice energy transfer below that at which fast electron decay channels open.

Fast electron emission through Coulomb induced recoil is predicted to be a dominant process, at lattice energy transfer where the nuclear recoil is strong enough for vacancy creation. There are currently relatively few reports of the observation of fast electrons in cold fusion expriments. Fast electron emission is predicted starting at relatively low energy transfer (a few KeV) from deuteron recoil, and at energies starting near 1 MeV for recoil from Pd. In the case of the stable Pd isotopes, this process competes with all beta decay reactions.

We have studied neutron transfer reaction mechanisms elsewhere[12,24,25] as a route to heat production. Although we have examined neutron transfers from ^{105}Pd to ^{6}Li, with an energy mismatch of 156 KeV, a more recent analysis suggests that this reaction will be suppressed due to selection rules affecting the Pd transition. There are new candidate reactions that are perhaps more promising relative to the selection rules: neutron transfer from ^{29}Si to ^{29}Si (producing ^{28}Si and ^{30}Si) at 2.14 MeV; and neutron transfer from ^{30}Si to ^{10}B at 845 KeV. In the case of the light water experiments, neutron transfer from ^{62}Ni to ^{29}Si has a mismatch of 12 KeV.

The generation of high phonon densities has not yet been addressed. We are considering seriously the possibility that D_2 desorption from the metal deuteride interface produces phonon gain when exothermic. In the case of PdD, the desorption is exothermic at high loadings,[26] which is correlated well with the proposed requirement of high PdD loading for heat production in Pons Fleischmann experiments. The quantum theories that have been developed for desorption[27,28] certainly contain all the essential physics for optical phonon gain, although this appears not to have been realized yet in the desorption literature. We will discuss this further elsewhere.

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