UNIFIED PHONON-COUPLED SU(N) MODELS FOR ANOMALIES IN METAL DEUTERIDES

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We present a systematic, but abbreviated, account of issues and models for anomalies in metal deuterides. To interact, deuterons must get close to one another, and we consider conditions under which this occurs and the ramifications. Within the general picture under discussion, anomalies are ultimately a consequence of phonon exchange that occurs when nuclear reactions take place in the solid state. We review the generalization of the resonating group method for reactions in vacuum to include solid state effects, and discuss implications for experiment. Phonon exchange in the case of a much simplified scalar Gaussian nuclear model is reviewed. The coupling of reactions at different sites is explored, and connections are made with recent experiments on alpha emission. The fastest site-other-site reactions are null reactions in which fusion reactions and their inverses are coupled. A consideration of these processes leads to the conclusion that compact states should be present stabilized by phonon exchange, and that these may be responsible for anomalies in recent beam experiments with metal deuterides. Energy exchange between nuclei and the lattice can be very efficient, according to results from idealized models for null reactions involving many sites. Aspects of excess heat production and other effects appear to be addressed by the new models.

1. Introduction

There has been considerable theoretical effort on the problem of anomalies in metal deuterides.[a] There exist some dated reviews of theoretical work,[1,2] but there has been no attempt in recent years to review work in this area generally. There is general agreement within the community that the excess heat effect is real, and that nuclear emissions occur. The evidence for ^{4}He production correlated with excess heat is compelling, and suggests that whatever is going on is consistent with an underlying d+d → ^{4}He reaction mechanism. Neither experiment nor theory has so far clarified how any of this works to the satisfaction of the community.

Recent theoretical work can be divided immediately into efforts that focus on reaction mechanisms consistent with d+d → ^{4}He, and other reaction mechanisms. With respect to the latter, Fisher has proposed reactions that involve polyneutrons,[3] and Kozima has written about neutron bands and neutron "drops".[4] With respect

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[a] For example, on the order of 70 abstracts on theoretical work were submitted for ICCF4.

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to the former, there are several different approaches currently being pursued that involve deuteron-deuteron reactions in some way. The possibility that the Coulomb interaction can be suppressed is being pursued by two efforts: Kim and coworkers[5] have written that quantum many-body effects may accomplish this; and S. R. Chubb and T. A. Chubb have argued that ion band state effects can lead to an effective reduction of the Coulomb interaction.[6,?] Li and coworkers have studied the possibility that resonant tunneling effects can account for some of the anomalies.[8] Hundreds of other works have been put forth that we have not mentioned in this brief discussion.

Most of the theoretical ideas put forth, including those cited above, have not been generally accepted as an explanation for the anomalies, and have not been pursued by other groups.[b] There are two approaches which have attracted some wider interest: these include the ideas of Takahashi, and of Preparata. Takahashi has written most recently about a proposed multi-deuteron resonant fusion scheme, in which three or more deuterons tunnel together in the metal deuteride.[9]

The general approach of Preparata is most closely related to the approach we have taken as discussed in this paper. Very much simplified, Preparata proposes that two deuterons make an electromagnetic transition to an intermediate nuclear state, and a second electromagnetic transition to the helium ground state.[10] The transitions in this three-state model are collective in the same sense as those described in our work. The electromagnetic interaction is coupled to electronic plasma modes in Preparata's approach. Preparata's ideas have attracted interest and support,[11] and remains an area of active research[12,13] following his loss before ICCF8.[14]

Our earliest efforts at developing models capable of predicting the fast reaction rates associated with the experimental claims were not particularly successful. After numerous failed attempts and many disappointments, we decided to focus instead on physical mechanisms, in the hope that understanding would emerge from a more fundamental point of view. A clear identification of the physical mechanisms involved might lead to incremental advances of connecting one piece of the puzzle at a time between theory and experiment. In the middle 1990s, this approach began to have the first minor successes in making connections between physical statements and experimentally observed effects. Incremental advances since that time have moved the models forward to their present form, where there now seem to be many connections to diverse experiments and effects. We believe that further effort along these lines will ultimately provide for a satisfactory theoretical understanding of the phenomena in general. In the sections that follow, we have made an attempt to give a systematic account of the different aspects of the models under development.

The starting place for our modeling at present is a pretty solid foundation that proposes that a description of nuclear processes in a metal deuteride should probably include the solid state environment at the outset in the formulation. Standard models from nuclear based on the application of vacuum physics models to metal

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[b]It has been remarked more than once among those working on anomalies in metal deuterides that all the theorists in the field are certain that the theories put forth by someone other than themselves are wrong.

deuterides will be successful in describing processes in which the solid state system interacts minimally. These do not include the new effects (low-level dd-fusion, energetic products not due to dd-fusion, heat and helium production, tritium production, and other anomalies), which from our perspective are a consequence of including the solid state in a fundamental way in the problem.

Although this manuscript is overly long for an ICCF proceedings paper, we are able to review only briefly a subset of the issues. Under such conditions, there is no possibility of adequately addressing issues properly. Consequently, we have made an attempt to isolate the main conjectures which have allowed us to make progress on the problem, and to spell them out simply and clearly. In this way, attention might be focused on the more important arguments and aspects of the models.

2. Maximization of the Deuteron-Deuteron Overlap

Certain specific aspects of different experimental results suggest that reactions involving two deuterons in the metal lattice occur. Examples of these include: (a) the reported observations of ^{4}He in proportion to the excess energy, with a reaction Q value of 24 MeV, consistent with a d+d $\rightarrow^4$He mechanism; (b) observations of dd-fusion reaction products at low levels and (c) observations of anomalies in metal deuterides with the absence of similar effects in metal hydrides. Consequently, we should be interested in the conditions under which two deuterons might come into close proximity so that they might react. This leads us to our first conjecture:

Conjecture I:

The probability that two deuterons will interact is maximized in the case of states involving double site occupancy of deuterium in a metal deuteride. Increasing the occupation of such states increases the reaction rate or the probability of reactions occuring.

2.1. *Maximization of the Overlap*

The argument in support of this conjecture can be presented in terms of an idealized model described by the Hamiltonian

$$\hat{H} \;=\; -\frac{\hbar^2\nabla_1^2}{2M} \;-\; \frac{\hbar^2\nabla_1^2}{2M} \;+\; V_{lat}(\mathbf{r}_1) \;+\; V_{lat}(\mathbf{r}_2) \;+\; V_{mol}(\mathbf{r}_2 - \mathbf{r}_1) \qquad (1)$$

This Hamiltonian describes two deuterons that are confined within a potential that extends over neighboring octahedral sites in a metal deuteride. Consider the ground state solution for the associated time-independent Schrödinger equation

$$E\Psi(\mathbf{r}_1,\mathbf{r}_2) \;=\; \hat{H}\Psi(\mathbf{r}_1,\mathbf{r}_2) \qquad (2)$$

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An approximate solution can be developed of the form[c]

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) \;=\; \sum_{i,j} \phi(\mathbf{r}_1 - \mathbf{R}_i)\phi(\mathbf{r}_2 - \mathbf{R}_j)g(\mathbf{r}_2 - \mathbf{r}_1) \tag{3}$$

where the ϕ functions are single deuteron wavefunctions and the $\mathbf{R}_i$ are the equilibrium positions in the octahedral sites. The separation function $g(\mathbf{r}_2 - \mathbf{r}_1)$ serves to keep the deuterons apart when they are in the same site.

The overlap probability in the special case that the two deuterons are assumed to be centered at neighboring sites in this approximation is

$$P_{ij}(\mathbf{r}) \;=\; V_{nuc}\,|\phi(\mathbf{r} - \mathbf{R}_i)|^2|\phi(\mathbf{r} - \mathbf{R}_j)|^2 g^2(0) \tag{4}$$

where V_{nuc} is a nuclear volume. The overlap probability when the two deuterons are at the same site is

$$P_{ii}(\mathbf{r}) \;=\; V_{nuc}\,|\phi(\mathbf{r} - \mathbf{R}_i)|^2|\phi(\mathbf{r} - \mathbf{R}_i)|^2 g^2(0) \tag{5}$$

The same-site overlap probability is maximized when the deuterons are both at the equilibrium position

$$P_{ii}(\mathbf{R}_i) \;=\; V_{nuc}\,|\phi(0)|^2|\phi(0)|^2 g^2(0) \tag{6}$$

To see how big the site-other-site overlap can be, we take the ratio of $P_{ij}(\mathbf{r})$ and the same site overlap at the equilibrium position

$$\frac{P_{ij}(\mathbf{r})}{P_{ii}(\mathbf{R}_i)} \;=\; \frac{|\phi(\mathbf{r} - \mathbf{R}_i)|^2}{|\phi(0)|^2}\frac{|\phi(\mathbf{r} - \mathbf{R}_j)|^2}{|\phi(0)|^2} \tag{7}$$

If we compute the ratio at a point $\mathbf{r}$ half-way between the two equilibrium sites, we find that a very small ratio is recovered, as the probability for tunneling to the half-way point is very small. A computation of the overlap probability near one of the equilibrium points is also very small, as one of the deuterons must tunnel all the way from one equilibrium point to the other. We conclude from this argument that two deuterons have the best chance of interacting if they occupy the same site.[d]

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[c]Much better approximate solutions can be developed in the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) \;=\; C\sum_{i \neq j} \phi(\mathbf{r}_1 - \mathbf{R}_i)\phi(\mathbf{r}_2 - \mathbf{R}_j)g(\mathbf{r}_2 - \mathbf{r}_1) \;+\; D\sum_i \psi(\mathbf{r}_1 - \mathbf{R}_i)\psi(\mathbf{r}_2 - \mathbf{R}_i)g(\mathbf{r}_2 - \mathbf{r}_1)$$

In this case, different single-particle wavefunctions are optimized when the two deuterons occupy the same site.

[d]It could be argued that a weakness of this argument is that the overlap probability for double occupation is on the order of that for molecular D_2 (as the two deuteron wavefunction is approximately molecular in this kind of model), and that the fusion rate which is well known for D_2 is too small to be relevant for any of the anomalies. However, in the models under consideration, a similar argument could be made based on taking the corresponding ratios of matrix elements instead of probabilities, and a similar conclusion would be reached.

2.2. *Connection with Experiment*

There are a variety of rather practical consequences that follow from this first conjecture. In no experiment has it been established directly that double occupancy states are occupied significantly, and hence there is no direct experimental connection between the occupation of such states and the occurrence of anomalies. But there is considerable indirect evidence, some of which we enumerate as follows:

(1) In Fleischmann-Pons experiments performed at SRI and elsewhere in the early 1990s, there appeared a correlation between the occurence of excess heat and high loading.[15] This is consistent with a requirement for deuterium in states of double occupancy, and we propose this as a more fundamental version of the requirement.

(2) It has been noted by several experimentalists that the excess heat effect is improved with increasing operating temperature.[e] Storms reported a measurement of the strong dependence of excess heat on temperature in a Fleischmann-Pon experiment, reporting it in terms of an activation energy through a statistical factor $(e^{-E/kT})$, with E serving as a chemical activation energy.[17] The energy is this measurement was about 670 meV. We propose that this temperature dependence is due in part to excitation to states of double deuterium occupation, with most of the 670 meV being associated with this particular kind of promotion.

(3) The activation energy for double occupancy is reduced in the presence of a single most metal atom vacancy. Metal lattices that are highly defective in this regard would be expected to be superior. This may be consistent with observations in the case of codeposition experiments and with the results of Case. Case recently gave results for his highly defective Pd catalyst on carbon, noting that the excess heat appeared to increase with temperature (from 185 C to 205 C) with an associated activation energy of 13 kcal/mol, which is about 560 meV.[18]

(4) Little in the models under discussion in this manuscript suggest that PdD is unique in the properties required for excess heat or other anomalies. Instead, it is the ability to load Pd very highly using electrochemistry near room temperature to achieve a high deuterium chemical potential that is more relevant in the Fleischmann-Pons experiment. Excess heat and other anomalies have been reported in a variety of other metal deuterides. In the Case experiment, the loading is not particularly high, yet there seems to be good evidence that excess heat is produced.

3. Site-other-site Reactions

Nuclear physics as currently understood in the mainstream literature and in textbooks does not provide a physical basis for the anomalies, as has been noted many times since 1989. Consequently, there must be new physical processes involved. Experimental results in which heat, or fusion products at low level, are observed are indicative that new physics is going on; but, in our view does not provide much insight as to precisely what physical mechanisms are involved. For this, we turn to experiments in which low-level nuclear products are seen that are not consistent with dd-fusion.

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[e]Fleischmann and Pons discussed a positive feedback mechanism early on,[16] which takes advantage in part of improved operation at higher temperature.

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In some experiments involving metal deuterides, fast alpha particles have been seen in relatively small amounts. In the case of PdD, alphas have been observed[f] between 11 and 16 MeV.[19] In the case of TiD, alphas and protons have been observed near 14 MeV.[20] We proposed previously that alpha emission above 10 MeV might occur based on a new kind of site-other-site reaction process, in which the energy from a reaction at one site is coupled to a reaction at another site.[22] We previously conjectured that site-other-site reactions of the form[23,24,25]

$$(d + d)_a \; + \; (^A\text{Pd})_b \; \longrightarrow \; (^4\text{He})_a \; + \; (^{A-4}\text{Ru} +^4 \text{He})_b \qquad (8)$$
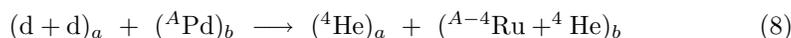
are involved in the production of fast alphas in the case of the PdD experiments. Below, we propose a modification of this kind of reaction, to be more consistent with the nuclear physics literature. Nevertheless, this leads us to our second conjecture:

Conjecture II:

It is possible for nuclear reactions at two sites to be coupled together as a second-order (or part of a higher-order) quantum process.

For this to be so, reactions at each site individually must exchange a quantum with some quantum system that has a coherence length which encompasses both sites. In the course of our investigations, we examined for this photon exchange, phonon exchange and interactions with plasmons. In the end, it seemed to be clear that phonon exchange would produce the largest effect of this sort, as phonon exchange in nuclear reactions would be mediated by the strong force, and hence be much stronger than processes involving photon exchange.

3.1. *Lattice Resonating Group Method*

Phonon exchange is usually not included in nuclear physics calculations of fusion processes. Our intuition about how nuclear reactions occur is based on a vacuum description, which was developed around 1930 and used successfully for nuclear physics work ever since. In this picture, a fast deuteron approaching a stationary deuteron in a metal deuteride might with some small probability tunnel to the stationary deuteron, approaching it on the fermi scale. If the two deuterons approach close enough to touch on the nuclear scale, then nuclear rearrangement can occur, and the exothermic nuclear products p+^{3}H or n+^{3}He leave about as fast as the laws of physics allows. Processes mediated by the strong force are no longer possible once the product nuclei are separated by about 10 fm, which occurs on a time scale on the order of 10^{-21} seconds. There is no time to communicate that a reaction has

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[f]We had been interested in some time by the report of Chambers et al,[21] as the alpha energies appeared to be consistent with a direct process in which the 24 MeV from the first site reaction is expressed in the alpha ejection. However, in that work there were noted diagnostic issues which cast doubt on the results. As these results have not been replicated, and as they are in qualitative disagreement with the results of Lipson et al,[19] we will disregard them.

happened with neighbors on the atomic scale before the reaction is over and done. Hence the reaction physics should be well described by a vacuum description. Detailed computations done using the resonating group method or R-matrix method, both vacuum models, give good agreement with experimental results.

Both the resonating group method and R-matrix method can be generalized to include phonon exchange with little difficulty, at least formally. In the case of the resonating group method,[26] we might write the variational wavefunction Ψ_t in the form

$$\Psi_t \;=\; \sum_j \Phi_j F_j \tag{9}$$

where the Φ_j keep track of the nuclear structure of the reactants, and the channel separation factors F_j describe the relative coordinates of the reactants. The optimization of the channel separation factors is accomplished through

$$E F_j \;=\; \langle \Phi_j | \hat{H} | \Phi_j \rangle F_j \;+\; \sum_{k \neq j} \langle \Phi_j | \hat{H} - E | \Phi_k F_k \rangle \tag{10}$$

The generalization of the resonating group method[24] can be accomplished by assuming a different variational wavefunction Ψ_t

$$\Psi_t \;=\; \sum_j \Phi_j \Psi_j \tag{11}$$

where the Ψ_j are lattice channel separation factors, which keep track of the separation of the reactants as well as the position of the other quantum particles in the relevant local environment. The optimization of the lattice channel separation factors is accomplished analogously

$$E \Psi_j \;=\; \langle \Phi_j | \hat{H} | \Phi_j \rangle \Psi_j \;+\; \sum_{k \neq j} \langle \Phi_j | \hat{H} - E | \Phi_k \Psi_k \rangle \tag{12}$$

With this generalization, we have an improved formulation that now includes phonon exchange, and contains earlier vacuum descriptions as a limit or subset. The new physics is compatible with earlier work in nuclear physics. This leads us to our third conjecture

Conjecture III:

The anomalies in metal deuterides can be accounted for theoretically within a formulation that generalizes the vacuum models to include the local solid state environment. No other new basic physics is required beyond what is in the textbooks, at least in principle.

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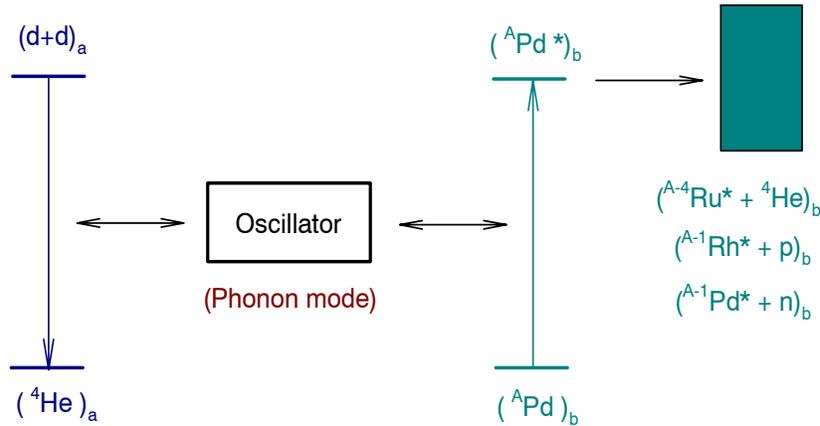
Figure 1. Schematic of an idealized second-order two-site reaction for the experiment of Lipson et al. Site-other-site coupling leads to the formation of a Bohr excited nuclear state in Pd, which decays through a multitude of channels (some of which are indicated).

There have been a wide variety of novel physical mechanisms proposed, including the possibility that quantum mechanics will need to be replaced, to account for the new experiments. In this conjecture, a belief is being expressed that only a single very plausible new piece of physics needs to be added to the large body of established physical law to make progress on this class of problem. In our work we have had much success proceeding in this way, but at this point we have no proof that this is so.

3.2. Connection with Experiment

Although the second-order site-other-site reaction mechanism under discussion is new, we would expect the alpha ejection part of the process to be something like photon-induced alpha emission, at least in the limit that a small number of phonons are exchanged. This latter process has been studied in the nuclear physics literature over the years, and at present is reasonably well understood. Photoalpha emission occurs primarily through a process in which an excited nucleus is formed, from which alphas and other particles evaporate.[27] There does exist a direct mechanism,[28] as we assumed in our earlier discussions, but this is at most a minor fraction of the total process. Photoalpha emission itself is only a small part of the total photoabsorption process. Most of the alpha particles within the statistical model are ejected at energies well below the maximum energy associated with a ground state to ground state direct process. Consequently, the signature of alpha ejection in the case of metal deuterides should instead be a broad distribution centered at energies below the maximum energy.[29] The resulting site-other-site mechanism is illustrated in Figure 1.
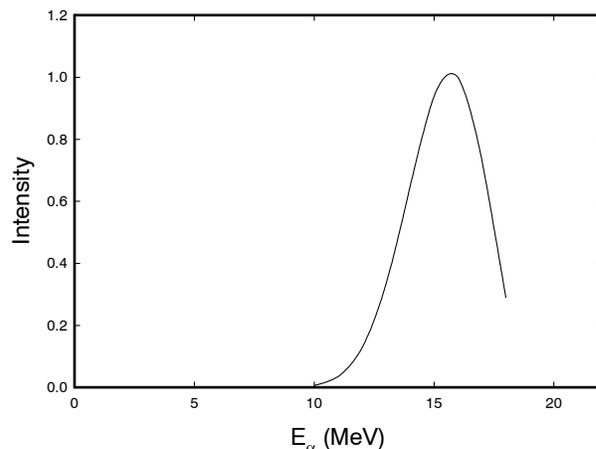
Figure 2. Spectrum for alpha emission estimate from a naive version of the Weisskopf-Ewing approximation.

(1) The observation of alphas in PdD in the range of 11-16 MeV of Lipson et al.[19] appears to be consistent with this kind of mechanism. We have estimated the alpha spectrum (see Figure 2) for this kind of mechanism from a naive version of the Weisskopf-Ewing model[27] based on

$$I(E) \sim e^{-2G(E)} E \, e^{(a\epsilon)^{1/2}} \tag{13}$$

with $\epsilon = \Delta E - I_\alpha - E$. This spectrum is a bit higher in energy than the experimental results. Note that a significant energetic proton signal would be expected below 14 MeV.

(2) The alpha and proton signals seen in TiD by Lipson et al.[20] is similarly consistent with the mechanism under discussion. The maximum proton and alpha energies for the different titanium isotopes is shown in Figure 3. We note that the alpha yield from photofission is larger in Ti than in Pd, which leads one to wonder whether the associated alpha signals in TiD through this mechanism would be larger than in PdD if all other things were equal.

(3) We note the measurements of energetic low mass charged ions from TiD by Cecil's group from the early 1990s, which is generally consistent with this kind of mechanism.[30]

(4) This kind of site-other-site disintegration mechanism should produce primarily neutrons and protons, with alphas, deuterons and tritons as having a lower integrated emission probability. Gammas would be present in connection with the stabilization of the daughter nuclei. In the case of neutron emission from a Bohr excited metal nucleus, a roughly exponential spectrum would be expected at low energy[31] (with a smaller contribution from the direct process). There exists at least one report of a roughly exponential neutron emission from TiD.[32]

It would be very interesting in future experiments to determine whether all of the expected particles and gammas are present in association with alpha emis-

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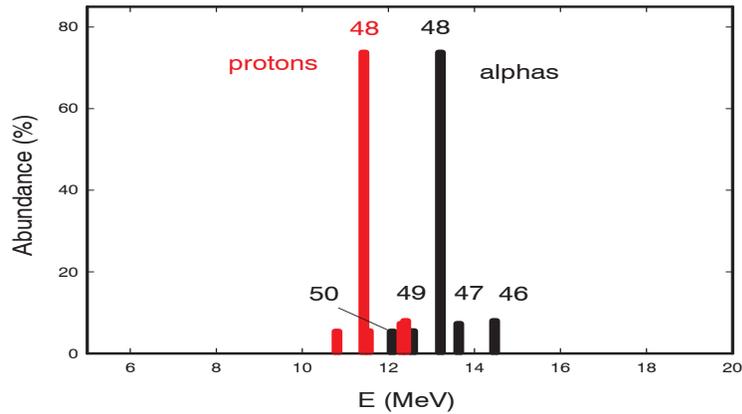
Figure 3.   Maximum proton and alpha ejection energies assuming $\Delta E = 23.85$ MeV.

sion, and to see whether the associated spectra can be compared with 24 MeV photodisintegration spectra.

3.3. *Not a Second-Order Process*

It is not difficult to develop a model for site-other-site coupling as a second-order process, such as outlined in previous work.[24] The computation is illuminating for two reasons. The first is that the resulting reaction rate is lower than experiment by tens of orders of magnitude, which leads immediately to the conclusion that this effect is not a simple second-order quantum process (present thinking is that it is a decay channel for the null reaction process discussed below). The second is that the computation illustrates clearly issues associated with localization. For models with thermal excitation, the off-resonant phonon field is localized, and there can be no effect. For a single highly-excited phonon mode with single phonon exchange at both sites, the effect is again local. However, for a single highly-excited phonon mode with nonlinear coupling at both sites, the second-order effect would be nonlocal. This is interesting, and it provides a foundation for nonlocality in the case of the null reactions.

4. Phonon Coupling

In the previous section, we described a formulation in which phonon interactions might be included at the outset in a fusion calculation. The resulting formulation is written in terms of lattice channel separation factors, which are much more complicated than the channel separation factors of the vacuum version of the problem. We have introduced a simplifying picture which allows for progress to be made on detailed calculations with the new model.

The basic issue is that the solid state quantum system has a large number of degrees of freedom, and it is prohibitive to attempt a computation in which an attempt is made to keep track of all of them. Hence we seek simpler models that contain the effects under discussion, but which neglect everything not essential. In this case, we propose an idealized model of the lattice in which a single phonon mode is highly excited, and all other phonon modes are excited thermally.[33] In the case of an individual lattice separation factor, this simplifying picture would allow us to work with approximate lattice channel separation factors of the form

$$\Psi_j \; \longrightarrow \; F_j \; \phi_n \qquad (14)$$

where ϕ_n is a simple harmonic oscillator eigenfunction describing n phonons in the highly-excited mode. All other modes are presumed thermal, and we suppress them in the notation.

There are numerous consequences of this, some of which will be touched on below. This leads us to yet another conjecture:

Conjecture IV:

Anomalies in metal deuterides are stimulated by strong phonon excitation.

The basic idea is that without strong phonon excitation, site-other-site interactions are suppressed, and the new processes under discussion do not occur. The issues of which phonon modes need to be excited, and by how much, remain to be addressed.

4.1. *Mechanism*

There are different approaches to the problem of phonon exchange mechanism. We recognize at least two different basic mechanisms. On the one hand, the positions of the center of mass of the different nuclei are phonon operators, and the strong force between nuclei can be thought of as a nonlinear interaction of very high order. On the other hand, if a reaction occurs then the phonon modes themselves may be different in the initial state reaction channel than in the final state reaction channel. An early description of this effect in the case of electronic transitions in molecules was given by Duschinsky.[34] There is no reason in principle why both mechanisms cannot play a role at the same time.

The two mechanisms lead to qualitatively different kinds of results in the analysis of anomalies in metal deuterides. The Duschinsky mechanism is far selective in what specific reactions are favored, and leads to perhaps a simpler picture overall. At present, our focus is on the Duschinsky mechanism.

Given a focus on Duschinsky coupling, the question that follows is what are the ramifications in the phonon-nuclear coupling problem. In molecular physics, a change in the phonon mode structure can result either from a change in the force constants or a change in the masses. From our perspective, if two deuterons are

localized within fermis, then to the lattice they will look like a helium nucleus, in terms of both force constants and masses.[g] On the other hand, transitions that result in a free neutron behave very differently, since the neutron is invisible to the lattice. For these transitions, a Duschinsky effect can be present since there is a mass change from the point of view of the lattice.

4.2. *Hybrid Description of Position Operators*

We have noted previously that there are difficulties inherent in the calculation of phonon-nuclear interactions since the nuclear interactions are localized and the phonon excitation is not. A description based on the nuclear center of mass coordinates $\hat{\mathbf{R}}_j$ is convenient for describing local interactions, but is highly inconvenient for describing a highly excited phonon mode. A description based on a decomposition into phonon operators $\hat{q}_m$

$$\hat{\mathbf{R}}_j \;=\; \mathbf{R}_j^0 \;+\; \sum_m \mathbf{u}_j[m]\,\hat{q}_m \tag{15}$$

is convenient for describing the highly excited phonon mode, but is highly inconvenient for describing local nuclear interactions. To resolve this issue, we have previously proposed a hybrid description of the form[35]

$$\hat{\mathbf{R}}_j \;=\; \mathbf{u}_j\hat{q} \;+\; \bar{\hat{\mathbf{R}}}_j \tag{16}$$

which isolates explicitly the contribution of the highly excited phonon mode $\mathbf{u}_j\hat{q}$, and combines the contributions from all the other phonon modes into a residual position operator $\bar{\hat{\mathbf{R}}}_j$.

4.3. *Phonon Interaction Matrix Element*

The discussion above allows us to begin estimating the phonon interaction matrix element. It is perhaps convenient here to examine the construction under the simplifying assumption of a scalar Gaussian nuclear model (with distinguishable nucleons), since this construction makes clear how the coupling works in this approach and allows for some initial quantitative estimates. We consider the specific example of phonon exchange in the case of a transition between the ^{4}He ground state and an n+^{3}He state.[h] We may write in the case of a particular interaction potential

$$V^{nn'}(\bar{\mathbf{r}}) \;=\; \langle\,\Phi[\mathrm{n}+^3\mathrm{He}]\,\phi_n \mid \hat{H} - E \mid \Phi[^4\mathrm{He}]\,\phi_{n'}\,\rangle \tag{17}$$

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[g]Although the force constants in this case may be very different upon separation.
[h]A detailed discussion of this kind of calculation has been given previously,[25,33] so here we focus on how the problem is set up initially.

We can think of this as a phonon matrix element in the sense

$$\langle\ \Phi[n+^3\text{He}]\ \phi_n\ |\ \hat{H}-E\ |\ \Phi[^4\text{He}]\ \phi_{n'}\ \rangle\ =\ \langle\phi_n|\hat{\Upsilon}(\overline{\mathbf{r}},\hat{q})|\phi_{n'}\rangle \tag{18}$$

where

$$\hat{\Upsilon}(\overline{\mathbf{r}},q)\ =\ \langle\ \Phi[n+^3\text{He}]\ |\ \hat{H}-E\ |\ \Phi[^4\text{He}]\ \rangle \tag{19}$$

where the integration is over the internal coordinates of the ^{3}He nucleus. Assuming a scalar Gaussian nuclear model,[i] we can take for the ^{4}He nucleus a wavefunction of the form

$$\Phi[^4\text{He}]\ =\ N_4\ e^{-\beta_4|\mathbf{r}_1-\mathbf{r}_2|^2}\ e^{-\beta_4|\mathbf{r}_1-\mathbf{r}_3|^2}\ e^{-\beta_4|\mathbf{r}_1-\mathbf{r}_4|^2}\ e^{-\beta_4|\mathbf{r}_2-\mathbf{r}_3|^2}\ e^{-\beta_4|\mathbf{r}_2-\mathbf{r}_4|^2}\ e^{-\beta_4|\mathbf{r}_3-\mathbf{r}_4|^2} \tag{20}$$

where N_4 is a normalization constant. For the n+^{3}He channel we take

$$\Phi[n+^3\text{He}]\ =\ N_3\ e^{-\beta_3|\mathbf{r}_1-\mathbf{r}_2|^2}\ e^{-\beta_3|\mathbf{r}_1-\mathbf{r}_3|^2}\ e^{-\beta_3|\mathbf{r}_2-\mathbf{r}_3|^2} \tag{21}$$

since there is no internal nuclear structure in this model associated with the neutron. We take for the interaction

$$\hat{H}-E\ \longrightarrow\ V_0\ [\ e^{-\alpha|\mathbf{r}_1-\mathbf{r}_4|^2}\ +\ e^{-\alpha|\mathbf{r}_2-\mathbf{r}_4|^2}\ +\ e^{-\alpha|\mathbf{r}_3-\mathbf{r}_4|^2}\ ] \tag{22}$$

where we assume a scalar Gaussian nuclear force of strength V_0.

4.4. *Evaluation of the Interaction*

Our interest in this model is in how the phonon interaction appears in the problem. The center of mass of the ^{4}He and ^{3}He nuclei (which are phonon position operators in the initial state and final states, respectively) are located at

$$\hat{\mathbf{R}}[^4\text{He}]\ =\ \frac{1}{4}[\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3+\mathbf{r}_4]\qquad \hat{\mathbf{R}}[^3\text{He}]\ =\ \frac{1}{3}[\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3] \tag{23}$$

The relative coordinates associated with the ^{3}He nucleus are

$$\mathbf{x}_1\ =\ \mathbf{r}_1-\hat{\mathbf{R}}[^3\text{He}]\qquad \mathbf{x}_2\ =\ \mathbf{r}_2-\hat{\mathbf{R}}[^3\text{He}]\qquad \mathbf{x}_3\ =\ \mathbf{r}_3-\hat{\mathbf{R}}[^3\text{He}] \tag{24}$$

Since $\mathbf{x}_1+\mathbf{x}_2+\mathbf{x}_3=0$, the integral of Equation (19) is over two of these coordinates. The coordinate $\mathbf{r}_4$ can be expressed in terms of the different center of mass coordinates according to

$$\mathbf{r}_4\ =\ 4\hat{\mathbf{R}}[^4\text{He}]-\mathbf{r}_1-\mathbf{r}_2-\mathbf{r}_3\ =\ 4\hat{\mathbf{R}}[^4\text{He}]-3\hat{\mathbf{R}}[^3\text{He}] \tag{25}$$

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[i]Gaussian models were once of interest in the nuclear physics literature in the 1930s.[36]

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The lattice channel separation factor is a function of the distance between the neutron and ^{3}He nucleus, which is a phonon operator

$$\hat{\mathbf{r}} \;=\; \mathbf{r}_4 - \hat{\mathbf{R}}[^3\text{He}] \;=\; 4\bigg(\hat{\mathbf{R}}[^4\text{He}] - \hat{\mathbf{R}}[^3\text{He}]\bigg) \;=\; \hat{\bar{\mathbf{r}}} \;+\; \Delta\mathbf{u}\,\hat{q} \tag{26}$$

We see a dependence of the phonon interaction in this problem on the relative position operator $\hat{\mathbf{R}}[^4\text{He}] - \hat{\mathbf{R}}[^3\text{He}]$, which will be nontrivial in this case since the transition involves a Duschinsky modification of the phonon mode structure due to a mass change. This was not present in the dd to ^{4}He matrix element that we considered before.[25] The $\hat{\Upsilon}$ operator can then be written in the form

$$\hat{\Upsilon}(\bar{\mathbf{r}}, \hat{q}) \;=\; V_0 N_3 N_4 \int d\mathbf{x}_1 \int d\mathbf{x}_2 \, e^{-\beta_3|\mathbf{x}_1-\mathbf{x}_2|^2} e^{-\beta_3|\mathbf{x}_1-\mathbf{x}_3|^2} e^{-\beta_3|\mathbf{x}_2-\mathbf{x}_3|^2}$$

$$\left[e^{-\alpha|\bar{\mathbf{r}}+\Delta\mathbf{u}\hat{q}-\mathbf{x}_1|^2} + e^{-\alpha|\bar{\mathbf{r}}+\Delta\mathbf{u}\hat{q}-\mathbf{x}_2|^2} + e^{-\alpha|\bar{\mathbf{r}}+\Delta\mathbf{u}\hat{q}-\mathbf{x}_3|^2} \right]$$

$$e^{-\beta_4|\mathbf{x}_1-\mathbf{x}_2|^2} e^{-\beta_4|\mathbf{x}_1-\mathbf{x}_3|^2} e^{-\beta_4|\mathbf{x}_2-\mathbf{x}_3|^2} e^{-\beta_4|\bar{\mathbf{r}}+\Delta\mathbf{u}\hat{q}-\mathbf{x}_1|^2} e^{-\beta_4|\bar{\mathbf{r}}+\Delta\mathbf{u}\hat{q}-\mathbf{x}_2|^2} e^{-\beta_4|\bar{\mathbf{r}}+\Delta\mathbf{u}\hat{q}-\mathbf{x}_3|^2}$$
$$\tag{27}$$

where $\mathbf{x}_3 = -\mathbf{x}_1 - \mathbf{x}_2$. The remaining computation for the scalar Gaussian model is straightforward. We see in the discussion above that the coupling between the nuclei and phonons appears in a natural way within the new formulation. Phonon exchange can introduce angular momentum on the microscopic scale, and result in a modification of the selection rules. Part of our research effort is currently aimed at upgrading the phonon coupling model to take advantage of more realistic nuclear wavefunctions and force models.[37]

4.5. *Connection with Experiment*

(1) Phonon exchange leads to the posibility of angular momentum exchange, which implies an ability to modify the microscopic angular momentum selection rules from the vacuum case. This lies at the heart of the possibility of d+d→^{4}He transitions without gamma emission, as part of site-other-site fast alpha emission, or in connection with excess heat production.

(2) There is at present no experimental result which demonstrates this mechanism cleanly in isolation. It may be possible to develop such an experiment. One possibility is low energy d+d reactions in a metal deuteride with a highly excited phonon mode, where phonon exchange would lead to a modification of the product angular distribution. Perhaps a better implementation is in the case of a p(n,γ)d reaction under conditions where the neutron and gamma momenta are matched, again assuming a highly excited phonon mode. When the neutron and gamma momentum are equal in magnitude and collinear, the emission in the absence of this effect will occur in a Mössbauer limit where no phonon exchange occurs.[38] Phonon exchange with a highly excited phonon field should be able to produce a modification in the resulting momentum matched angular distribution.

(3) In the discussion that follows we will be interested in conditions under which 20 or more units of angular momentum are exchanged through this mechanism in association with excess heat production. We estimated previously that a criterion for this is that the displacement of helium nuclei in relevant sites due to a single highly excited phonon mode should be on the order of 100 fm (independent of the phonon mode frequency). Consequently, we are interested in the issue of how such phonon excitation is developed in different experiments to initiate an excess heat effect. We have proposed previously that this can be accomplished by driving a deuterium flux inside the metal deuteride down a sharp chemical potential step (which might be present inside the metal between different regions, in the vicinity of layers of different materials, or in the case of exothermic desorption of a highly loaded PdD sample). Evidence in support of this comes from the existence of a current threshold in association with the excess heat effect, with the associated interpretation that only when the threshold is reached is there sufficient phononic excitation to transfer 20 or more units of angular momentum.

5. Null Reactions

If there can be new site-other-site reactions, as implied by the fast alpha experiments, the question might be asked as to what the fastest reaction of this kind might be, considering all possible atomic and nuclear mechanisms. Our initial speculation was that in the case of an initial phonon-coupled fusion process of the form $d+d \rightarrow$ ^{4}He (which we considered because of its implication in fast alpha emission), that the reaction rate would be fastest if coupled to the inverse process. In the case of a two-site reaction process, this would produce a reaction of the form

$$(d + d)_a \; + \; (^4\text{He})_b \; \longrightarrow \; (^4\text{He})_a \; + \; (d + d)_b \tag{28}$$
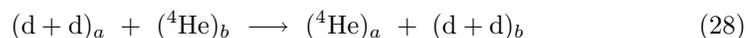
The original proposal involved phonon exchange at both sites, both to satisfy the microscopic selection rules and also to provide a mechanism for coupling the reactions together. In light of the discussion in the previous section, our simplistic notion of the null reaction is probably useful for pedagogical purposes, but would not correspond precisely to the microscopic physics since the individual transitions do not involved phonon exchange through a local Duschinsky mechanism.

In the initial analysis of this process it appeared that localized states might be produced. The initial argument was that as the Coulomb barrier inhibited tunneling in the case of deuterons tunneling initially from an atomic scale separation, the same Coulomb barrier should inhibit tunneling to an atomic scale separation. Our initial calculations seemed to support this notion, as long as transitions between several sites occured. Our current point of view has led to a more complicated picture, in which both the null reaction and the compact states are present, but as part of a more complex process. In this picture, initial transitions from D_2 states associated with double site occupancy would go initially to compact n+^{3}He states, thus satisfying the requirement for a Duschinsky transition. Compact n+^{3}He states

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would undergo transitions to ^{4}He states,[j] and it is these transitions which would be important in stabilizing the compact states. This leads us to our next conjecture:

Conjecture V:

Null reactions are the dominant processes of the new phonon-coupled site-other-site reactions in metal deuterides.

As presently conceived, the most important and fastest of these are phonon-induced transitions between helium nuclei and compact n+^{3}He states in metal deuterides.

5.1. *The Two-Site Problem*

The simplest model that we can formulate that illustrates how site-other-site interactions might work within the new theory is the two-site problem. We proposed a version of this model earlier,[25] in the context of null reactions based on d+d→^{4}He transitions. Since that time our point of view has changed some, and our focus now is on different aspects of the model. In the case of a simple scalar nuclear physics model, the two-site problem can be studied using a trial wavefunction of the form

$$\Psi_t = \sum_n A_n \left| \Phi^a[^4\mathrm{He}] \, \Phi^b[^4\mathrm{He}] \, \phi_n \right\rangle + \sum_{nlm} \left| \Phi^a[\mathrm{n}+^3\mathrm{He}] \, \Phi^b[^4\mathrm{He}]^b \, \phi_n \, Y_{lm} \right\rangle \frac{P^a_{nlm}(r)}{r}$$

$$+ \sum_{nlm} \left| \Phi^a[^4\mathrm{He}] \, \Phi^b[\mathrm{n}+^3\,\mathrm{He}] \, \phi_n \, Y_{lm} \right\rangle \frac{P^b_{nlm}(s)}{s}$$

$$+ \sum_n \sum_{lm} \sum_{l'm'} \left| \Phi^a[\mathrm{n}+^3\,\mathrm{He}] \, \Phi^b[\mathrm{n}+^3\,\mathrm{He}] \, \phi_n \, Y^a_{lm} \, Y^b_{l'm'} \right\rangle \frac{P^{ab}_{nlml'm'}(r,s)}{rs} \quad (29)$$

The optimization of the lattice channel separation factors in this case leads to coupled-channel equations which are provided in the Appendix. Our interest previously was in the question of whether the two-site problem permitted stable bound state solutions, and if so whether the associated wavefunctions could be found. Although this question remains of interest to us, there are other issues that might profitably be considered.

A useful concept for a class of problems in quantum mechanics is the notion of a leaky well and nearly bound states. If one has a finite well with finite barriers, it may be possible to develop approximate bound states of the well. Since we have assumed that the barriers are finite, this approximate bound state will leak out of the well with a decay time that could be estimated through standard techniques. It would then be possible to use these unstable states as approximate basis states to calculate the dynamics (and other properties) of a particle within the lossy well.

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[j]Also transitions to p+t states, but this will be of interest later.

If we restricted our attention to the region inside the well, then we could make much progress from a knowledge of the nearly bound state energy, wavefunction, and decay rate. A finite basis description for the probability amplitude within the well could be developed in the form

$$\psi(\mathbf{r}, t) \;=\; \sum_j \, c_j(t) u_j(\mathbf{r}) \tag{30}$$

The expansion coefficients would satsify and equation of the form

$$i\hbar\frac{d}{dt}\mathbf{c}(t) \;=\; \mathbf{H} \cdot \mathbf{c}(t) \;-\; \frac{i\hbar}{2}\mathbf{\Gamma} \cdot \mathbf{c}(t) \tag{31}$$

If the basis states u_j are approximately eigenfunctions within the well, then the matrix $\mathbf{H}$ will be approximately diagonal with the nearly bound state energy eigenvalues. In this case the approximately diagonal matrix $\mathbf{G}$ would contain the decay rates for the different nearly bound states.

We can use this picture in connection with the two-site problem (or with many-site problems as well). Associated with each channel in the coupled-channel equations we could assign a localized basis state which could in principle be optimized. Associated with each basis state an energy could be estimated (including kinetic and potential terms, but not including source terms). An estimate for the decay rate could be obtained (although there are probably elegant ways to do this, if all else fails one could solve for the rate of probability loss channel by channel when source terms are present). In the end, what is of interest in the development of a lossy matrix equation is a collection of energies, decay rates, and coupling matrix elements for the localized basis states in all of the channels.

The outcome of this kind of model is a variety of conclusions, most of them obvious. We find that localization increases the kinetic and centripetal energy terms, and that the degree of localization is determined by the nuclear interaction terms with phonon exchange $v_{lm}^{nn'}$ – which depends on the maximum relative displacement $|\Delta\mathbf{u}q_{max}|$, assuming that n is large. We also find that the decay rates go down with increasing angular momentum l, and that the range of angular momentum l produced again depends on the maximum relative displacement $|\Delta\mathbf{u}q_{max}|$ and the number of phonons exchanged. We can think of the localized finite basis expansion in this case as being of the form

$$\Psi \;=\; \sum_n \sum_j \, c_{j,n}(t) \, u_j \, \phi_n \tag{32}$$

The coefficients $c_{j,n}(t)$ would then satisfy an equation of the form

$$i\hbar\frac{d}{dt}\mathbf{c}_n(t) \;=\; \mathbf{H}_n \cdot \mathbf{c}_n(t) \;+\; \sum_{n'}\mathbf{V}_{nn'} \cdot \mathbf{c}_{n'}(t) \;-\; \frac{i\hbar}{2}\mathbf{\Gamma}_n \cdot \mathbf{c}_n(t) \tag{33}$$

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We end up with a potentially complicated description of the dynamics where the state energies, decay rates and coupling matrix elements all come into play. Although we have investigated a variety of approaches and approximations for the solution of the two-site problem, we do not have in hand solutions at present. The consideration of this problem has nevertheless taught us much about how to think about this kind of problem, how to begin to approach problems where more sites are involved, and also what kinds of simpler models might be relevant and illuminating about such problems. Our conclusion from these studies so far is that when sufficient angular momentum transfer occurs, the centripetal barrier inhibits tunneling and the associated decay rates become very small. In this limit, we think it quite probable that rather stable compact states result in the case of the many-site version of the problem. This leads us to the following conjecture:

Conjecture VI:

Null reactions in metal deuterides can result in stable compact states when sufficient phonon exchange occurs so that on the order of 20 or more units of angular momentum are exchanged.

5.2. *Connection with Experiment*

(1) The stabilization of localized states through angular momentum exchange in association with phonon exchange is a very interesting possibility in addressing the problem of how the new proposed phonon-nuclear reactions might compete against the very fast conventional d+d reactions. If a high centripetal barrier is present, then the conventional d+d reactions can be slowed down by tens of orders of magnitude.

(2) Kasagi has reported the observation of unexpected fast proton and fast alpha signals that he has conjectured are due to a three-body reaction[41]

$$d \; + \; d \; + \; d \; \longrightarrow \; n \; + \; p \; + \; {}^4He$$

For such a reaction to occur, a single deuteron would need to come into contact with two deuterons that are within roughly 10 fermis, which is exceedingly unlikely without new physics. We have conjectured that these experiments may be interpreted as detecting two-body compact states as discussed in the section above.[42] The compact states in this case would originate from deuterons in states of double occupancy in the metal deuteride, and hence have energies close to the two deuteron energy.

The number of compact states consistent with Kasagi's measurements, and also with similar experiments done recently at NRL,[43] is on the order of 10^{-6} of the deuterons present in the near-surface part of the lattice. Such a large number of compact states would lead to very high rates of conventional dd-fusion products unless there was some mechanism to stabilize the compact states. Estimates of the phonon exchange potentials suggest that it is relatively easy for significant angular momentum exchange to occur when many phonons are exchanged, suggesting that the compact states may have high angular momentum. The centripetal barrier present when there are on the order of 20 units of angular momentum or more is

sufficient to suppress the tunneling of fusion reaction products. Support for this conjecture comes from the relative absence of products from the two-body reaction channel in these experiments

$$d + d + d \longrightarrow d + {}^4He$$
$$d + d + d \longrightarrow t + {}^3He$$
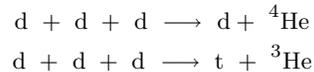
The relative absence of the two-body exit channels is consistent with the presence of significant angular momentum in the compact state.

(3) Information about the degree of localization of the compact state could in principle be obtained in Kasagi experiments in which the incident deuteron energy is varied.

(4) Information about the amount of angular momentum present could in principle be obtained using a different incident particle for which only two-body reaction products are available. In this case, conservation of angular momentum would require that the incident particle would need to contribute angular momentum in order to open channels with reduced angular momentum (and hence centripetal potential).

(5) A interesting and important question is whether compact states might exist in the case of the p+d system. One might expect a Duschinsky phonon exchange mechanism to be available for compact p+p+n localized states.

6. Energy Exchange between Nuclei and Phonons

One of the most difficult things to accept in the initial claim of the Fleischmann-Pons effect was the possibility of converting nuclear quanta to heat in the absence of fast ions or neutrons. This issue has been of major concern in our studies over the past 15 years. In recent years we have favored models in which the energy exchange occurs a few phonon quanta at a time in association with a large number of very fast reactions. Our next conjecture is concerned with this issue:

Conjecture VII:

If sufficient angular momentum exchange occurs so as to stabilize the compact states, then the phonon exchange that occurs in association with null reactions couples energy effectively between nuclear and phononic degrees of freedom.

6.1. *Phonon-Coupled SU(3) Model*

In our discussion of the two-site model, we ended up with many lossy nuclear states coupled to potentially many states of a highly-excited phonon mode, and an associated matrix description given by Equation (33). To begin trying to understand the physical content of that model and more complicated models involving interactions between many sites, we turn our attention to much simpler toy models which seek to retain important features of the full model but are easier to analyze and to

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understand. The simplest possible model that has the potential of being relevant to this problem is the phonon-coupled SU(3) model. In this model, we assume that at a given site we may have three different kinds of states: deuterons with double occupancy, compact n+^{3}He states, and ^{4}He ground states. Transitions between compact states and ^{4}He states occur with a large interaction strength, and occurs with enough phonon exchange to stabilize the compact states. Transitions between deuteron states and compact states occurs with a much weaker interaction due to the poor overlap between the molecular wavefunction associated with double occupancy and the compact nuclear states. All sites are assumed to interact uniformly with the highly excited phonon mode. The associated Hamiltonian is

$$\hat{H} = E_{^4\text{He}} \sum_j \begin{pmatrix} 0\ 0\ 0 \\ 0\ 0\ 0 \\ 0\ 0\ 1 \end{pmatrix}_j + E_{com} \sum_j \begin{pmatrix} 0\ 0\ 0 \\ 0\ 1\ 0 \\ 0\ 0\ 0 \end{pmatrix}_j + E_{mol} \sum_j \begin{pmatrix} 1\ 0\ 0 \\ 0\ 0\ 0 \\ 0\ 0\ 0 \end{pmatrix}_j + \hbar\omega_0 \left(n + \frac{1}{2} \right)$$

$$+\ e^{-G} \sum_j \sum_{n'} V_{nn'} \hat{\delta}_{nn'} \begin{pmatrix} 0\ 1\ 0 \\ 1\ 0\ 0 \\ 0\ 0\ 0 \end{pmatrix}_j + \sum_j \sum_{n'} U_{nn'} \hat{\delta}_{nn'} \begin{pmatrix} 0\ 0\ 0 \\ 0\ 0\ 1 \\ 0\ 1\ 0 \end{pmatrix}_j \qquad (34)$$

The energies of the different nuclear states $E_{^4\text{He}}$, E_{com}, and E_{mol} correspond to ^{4}He states, compact states, and two-deuteron molecular (double occupancy) states within the metal deuteride, respectively. The phonon energy is $\hbar\omega_0$. The tunneling of two deuterons from the atomic scale to the nuclear scale is accounted for through the tunneling factor e^{-G}. The nuclear interaction strengths are denoted by U and V, with phonon exchange accounted for by $\hat{\delta}_{nn'}$ operators. This model is assumed to be augmented by additional decay matrix $\boldsymbol{\Gamma}$ which accounts for the decay of unstable localized states where energetically and kinematically allowed.

Studies that we have done so far indicate that in the absence of loss terms, there is little energy transfer between the nuclear and phononic degree of freedom under conditions where there are a great many phonons present and states with large Dicke numbers are used. The presence of loss terms breaks the underlying symmetry within the system, and leads to reasonably free transfer of energy between the two degrees of freedom. The conditions under which this occurs was found to be when roughly 15 or more compact states and helium nuclei were present, assuming that sufficient angular momentum transfer occurs to stabilize the compact states.[25] If insufficient angular momentum is present in the compact states, then they decay through the conventional dd-fusion channel prior to losing energy to the phonon mode. Our studies so far support the conjecture above.

6.2. Connection with Experiment

(1) The phonon-coupled SU(3) model sheds light on how nuclear energy can exchange with phonon energy, and indicates that there may be some merit to Fleischmann's conjecture of a new physical process that accomplishes d+d→^{4}He with the excess energy going into heat. Experimental observations of ^{4}He in connection with excess energy measurements[44] indicates a reaction Q value in the range of 24 MeV, in agreement with the theoretical expectation.

(2) Within the phonon-coupled SU(3) model an excess heat effect would be expected at high angular momentum exchange, whereas other decay modes (such as dd-fusion) would be dominant at lower angular momentum exchange. If we accept a connection between the electrochemical current density and the strength of phonon excitation, then we might expect from this kind of model low level fusion products at low current density but no excess heat, and excess heat at high current density but no dd-fusion products. In the early 1990s it was noted that there was great similarities between the electrochemical experiments run by K. Wolf in association with neutron measurements,[45] and those of the SRI group in association with excess heat measurements. Perhaps the most important difference was in the current density used. In the Wolf experiments, the preliminary cathode charging was done at 20 mA/cm^2, and evidence for neutron emission was obtained at an elevated current density of 30 mA/cm^2 (and according to Wolf, the range of current densities in which neutron emission was observed was relatively narrow). In the SRI experiments,[39] the excess heat effect appeared to turn on at a current threshold in the range of 200-300 mA/cm^2. If we propose that the angular momentum transfer in these experiments is proportional to the square root of the current density, then we conclude that neutron emission is produced at an angular momentum exchange a factor of three below that required for the onset of excess heat. This is qualitatively in agreement with the models under discussion (it is not yet known if there is quantitative agreement).

(3) The models under discussion convert nuclear energy to phonon energy in the mode that caused the interactions in the first place. This is much like the case of stimulated emission in lasers, where the atomic transition energy goes into the modes of the photons that caused the transition. In this case, the model describes a rather strange kind of nonlinear phonon laser. The metal deuteride is the phonon gain medium. When the phonon amplitude is made sufficiently large to initiate reactions, then lasing occurs. Once the system is inputting energy into the highly excited phonon mode, it may be able to self sustain. This notion is reflected in excess heat experiments that show a "heat after death" effect, in which power input is removed but excess heat production is sustained.[40]

7. Slow Tritium Production

There have been many reports of slow tritium production in experiments with metal deuterides since 1989.[46] The tritium produced in these experiments is generated in the absence of neutrons, so it is not due to the conventional d+d → p+t reaction pathway. Moreover, neutron measurements performed in association with tritium production indicate that there is an absence of 14 MeV neutrons that would be associated with d+t → n+^{4}He reactions.[47] The relative absence of neutrons implies that the tritium must be born slow, and measurements allow for an upper limit of triton energy to be estimated at about 10 keV.[48]

The models under discussion appear to be relevant to slow tritium production. Within the general framework under discussion, slow tritium production appears as a consequence of the inclusion of p+t double occupancy. This leads to the conjecture

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Conjecture VIII:

Slow tritium production in metal deuterides is a consequence of tunneling from the compact state population to a double occupancy (molecular) HT state within the metal deuteride. A similar mechanism is not present for tunneling to $n+^3He$ states as the neutron does not remain localized.

7.1. *Phonon-Coupled SU(4) Model for Tritium Production*

The simplest possible model that appears to be relevant to tritium production is the phonon coupled SU(4) model. The associated Hamiltonian is given by

$$
\hat{H} \;=\; E_{^4\mathrm{He}} \sum_j \begin{pmatrix} 0\,0\,0\,0 \\ 0\,0\,0\,0 \\ 0\,0\,0\,0 \\ 0\,0\,0\,1 \end{pmatrix}_j + E_{\mathrm{t+p}} \sum_j \begin{pmatrix} 0\,0\,0\,0 \\ 0\,0\,0\,0 \\ 0\,0\,1\,0 \\ 0\,0\,0\,0 \end{pmatrix}_j + E_{com} \sum_j \begin{pmatrix} 0\,0\,0\,0 \\ 0\,1\,0\,0 \\ 0\,0\,0\,0 \\ 0\,0\,0\,0 \end{pmatrix}_j
$$

$$
+\; E_{mol} \sum_j \begin{pmatrix} 1\,0\,0\,0 \\ 0\,0\,0\,0 \\ 0\,0\,0\,0 \\ 0\,0\,0\,0 \end{pmatrix}_j \;+\; \hbar\omega_0 \left(n + \frac{1}{2} \right) \;+\; e^{-G} \sum_j \sum_{n'} V_{nn'} \hat{\delta}_{nn'} \begin{pmatrix} 0\,0\,1\,0 \\ 0\,0\,0\,0 \\ 1\,0\,0\,0 \\ 0\,0\,0\,0 \end{pmatrix}_j
$$

$$
+\; e^{-G'} \sum_j \sum_{n'} W_{nn'} \hat{\delta}_{nn'} \begin{pmatrix} 0\,0\,0\,0 \\ 0\,0\,1\,0 \\ 0\,1\,0\,0 \\ 0\,0\,0\,0 \end{pmatrix}_j \;+\; \sum_j \sum_{n'} U_{nn'} \hat{\delta}_{nn'} \begin{pmatrix} 0\,0\,0\,0 \\ 0\,0\,0\,0 \\ 0\,0\,0\,1 \\ 0\,0\,1\,0 \end{pmatrix}_j \tag{35}
$$

The basic idea here is to recognize that double occupancy of a participating site with HT should be included within the scheme on equal footing to double occupancy with D_2, and that no similar construction is possible for the $n+^3$He channel. Experimental observations of tritium production within neutron detectors have indicated an absence of fast neutrons in association with the tritium. In this model reacting deuterons in the lattice give up their energy to phonons, and produce bound HT in double occupancy. Consideration of this kind of model to date suggest that tritium production may occur in a regime in which insufficient energy transfer occurs to reach ^{4}He, and where protons and tritons are present initially in the metal deuteride.

7.2. *Connection with Experiment*

(1) The existence of a clear pathway for tritium production within the model that is much like the pathway for excess heat production, but comes without an equivalent $n+^3$He pathway is in qualitative agreement with the experimental results.[46,47]

(2) The model predicts that there should be an excess heat effect in association with tritium production. No such effect has been detected experimentally yet.

(3) The models under discussion suggest the possibility of an exclusion effect between heat and tritium production. The idea is that under conditions of very strong

coupling, the compact state probability amplitude will simply bypass the tritium channel tunneling exit. If coherence factors are important as we expect, then whatever process starts first will be reinforced leading to an exclusion of the other. If this line of argument is right, then one would expect there to be a current threshold for tritium production that lies between the threshold for neutron production and excess heat production.

8. Dynamics, Tunneling, and Coherence

One of the most difficult things to theoretical models to address in association with the experimental results is the tremendous acceleration of the tunneling process between deuterons which is implied by the relatively fast reaction rates. There have been (and there continue to be) efforts to account for this through enhancements in screening due to one mechanism or another. We have concluded that there is no reasonable physical basis for screening enhancements as large as would be required to be consistent with the slowest of the low-level fusion reaction claims.[49] Moreover, an enhancement of the screening does not help make progress on other important apsects of the outstanding theoretical issues.

It is known that the dynamics would be modified significantly if there were a localized nuclear state with an energy resonant with the two deuteron state, and if decoherence could somehow be ignored. In this case, the mathematical solutions involve Rabi oscillations between the resonant atomic scale and nuclear scale states, with greatly enhanced tunneling.[50] Although there is no stable resonant four nucleon state in vacuum with the right energy (and there is no way to suppress decoherence), we recognize this model as being important nevertheless. It makes clear the difference between tunneling as part of an incoherent process, where the reaction rate is proportional to the square of the matrix element (and the tunneling is proportional to e^{-2G}); and tunneling as part of a coherent process, where the reaction rate is linear in the matrix element (and the tunneling is proportional to e^{-G}). The existence of this idealized resonant tunneling model suggests that we should seek theoretical models in which the tunneling comes in coherently, and that this effect is ultimately the source of the great acceleration in tunneling. This leads us to the conjecture:

Conjecture IX:

Tunneling between deuterons (or other nuclei) can occur in connection with other fast processes that are coherent, such that the associated rate is linear in the tunneling factor e^{-G}.

Models where tunneling comes into the calculation with a dependence of the form e^{-2G} do not lead to reaction rates that are commensurate with experimental claims.

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8.1. *Adiabatic Approximation*

To examine this issue, we examine the dynamics associated with the phonon-coupled SU(3) model as a representative example of more general models consistent with Equation (33). The phonon-coupled SU(3) model includes processes that are very fast (exchange between the compact states and ground state helium levels) and processes that are very slow (tunneling from the molecular states to the compact states). Consequently, one might expect a separable approximation to be relevant, in which the fast processes "equilibrate" on a time scale much shorter than the tunneling. In this case, we propose an approximate solution of the form

$$\Psi \;=\; \sum_N \sum_j c_{N,j}(t)\, u_{N,j} \tag{36}$$

where N is the number of sites with molecular state occupation. The basis states $u_{N,j}$ satisfy

$$\left(E_{N,j} - \frac{i\hbar}{2}\gamma_{N,j}\right) u_{N,j} \;=\; \left(\hat{H}_0 - \frac{i\hbar}{2}\hat{\Gamma}\right) u_{N,j} \tag{37}$$

where $\hat{H}_0$ includes all terms in the phonon-coupled SU(3) Hamiltonian of Equation (34) except those associated with tunneling. The dynamics of the system in this approximation follow from evolution equations of the form

$$i\hbar \frac{d}{dt} c_{N,j}(t) \;=\; \left(E_{N,j} - \frac{i\hbar}{2}\gamma_{N,j}\right) c_{N,j}(t) + \sum_k \langle v_{N,j}|\hat{V}|u_{N+1,k}\rangle\, c_{N+1,k}(t)$$

$$+ \sum_k \langle v_{N,j}|\hat{V}|u_{N-1,k}\rangle\, c_{N-1,k}(t) \tag{38}$$

In this equation $\hat{V}$ includes tunneling terms from Equation (34), and the $v_{N,j}$ are the adjoint functions associated with the $u_{N,j}$.

We see immediately a need for the decay rate $\gamma_{N,j}$ of the eigenstates to be small as a prerequisite for any coherent dynamics. We have remarked above on the need for large angular momentum exchange to stabilize the compact states. There is an additional effect present which we observed in the computations discussed in previous work,[25] where we found that the probability amplitude in the quantum flow calculation avoided states with significant loss. Due to the close connection between those computations and the lossy eigenfunction calculation here, the same effect occurs in this problem and is greatly helpful in stabilizing the eigenfunctions.

8.2. *Limiting Case with a Simple Resonance*

Models of complicated quantum systems can exhibit a wide variety of effects, and one usually seeks to focus on states or limiting behavior where the specific effects of

interest are brought out cleanly. In this case, we are interested in specific solutions which exhibit rapid accumulation of compact states from states with deuteron pairs in double occupancy. The simplest example of this is in the case of the phonon-coupled SU(3) model where we assume that the compact state is resonant with the molecular state within the metal deuteride.[k] In a highly idealized model of this kind, where we assume that the angular momentum exchange is sufficiently great to stabilize the compact states so that the associated γ can be neglected, we would obtain

$$i\hbar\frac{d}{dt}c_N(t) \;=\; Ec_N(t) \;+\; \langle v_N|\hat{V}|u_{N+1}\rangle \, c_{N+1}(t) \;+\; \langle v_N|\hat{V}|u_{N-1}\rangle \, c_{N-1}(t) \quad (39)$$

In this limit we are able to obtain approximate solutions that are sinusoidal with an associate Rabi oscillation frequency on the order of $\dfrac{V_0 e^{-G}}{\hbar}$ per deuteron pair in states of double occupancy. We are at once pleased that the phonon-coupled SU(3) model is capable in some limit of producing an enhanced tunneling effect, but discouraged because the resulting reaction rate is a few orders of magnitude less than what is needed to be relevant for experiments in which excess heat is observed.

8.3. *Limiting Case with Interaction between Coherent Populations*

The physical picture that corresponds to the idealized model above is one in which deuterons at the atomic scale tunnel to produce a local resonant stable compact state at the same site. Nuclear energy is converted to phononic energy subsequently, the dynamics of which are assumed to be fast and accounted for in the u_N eigenfunctions. We can think of this limit of the model as being closely related to the idealized single-site resonant tunneling model outlined above, and the resulting reaction rates and dynamics are the same as for the single site model in regard to the tunneling.

It should be noted that there is another rather general kind of behavior that might be expected for models that include more compact state levels than the phonon-coupled SU(3) model. Consider a model in which tunneling initial leads to a compact state that is not resonant, but involves an energy defect that might be considerable. Let us suppose that this energy defect is balanced by transitions at other sites from a compact state at one energy to one at another energy that precisely balances the energy defect to bring the system back to resonance. In this case, the dynamics associated with an idealized model that focus on this effect would be of the form

$$i\hbar\frac{d}{dt}c_N(t) \;=\; Ec_N(t) \;+\; \langle v_N|\hat{V}'|u_{N+1}\rangle \, c_{N+1}(t) \;+\; \langle v_N|\hat{V}'|u_{N-1}\rangle \, c_{N-1}(t) \quad (40)$$

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[k]Such a precise matching seems to be unlikely, but we recall that the energies of the compact states will depend on the amplitude of the excited phonon mode, which suggests that there is a possibility of a feedback mechanism which might lead to a locking of the compact state energy.

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where $\hat{V}'$ is of the form

$$\hat{V}' \;=\; e^{-G} \sum_{n'} V_{nn'} \hat{\delta}_{nn'} \; \left(\hat{\Sigma}_+^{(1)} \hat{\Sigma}_-^{(2)} \;+\; \hat{\Sigma}_-^{(1)} \hat{\Sigma}_+^{(2)} \right) \tag{41}$$

where the $\hat{\Sigma}_{\pm}$ operators are pseudostate raising and lowering operators for the two systems.

The dynamics associated with this kind of model behave very differently than for the resonant SU(3) model discussed above.[50] This model describes a new situation in which the collective tunneling transitions at all participating sites of double occupancy interact uniformly with collective balancing transitions among compact states at all of their participating sites. In essence, one population is interacting collectively, as a population, with another population that is responding collectively, also as a population. The dynamics associated with this kind of process can be much faster, with a peak rate that is on the order of $\sqrt{N_1 N_2} \dfrac{V_0 e^{-G}}{\hbar}$ per deuteron pair in states of double occupancy, where N_1 and N_2 are connected with the Dicke numbers of the individual transitions. The associated dynamics exhibit a "burst" type of behavior, which is characteristic of superradiant systems (the discussion here is concerned with a Dicke type enhancement of a coherent quantum process, instead of incoherent processes such as superradiant radiative decay). This discussion leads us to our final conjecture:[1]

Conjecture X:

The coherent tunneling process can be enhanced by a phase coherence between transitions at different sites, producing a superradiant enhancement.

We have considered here an idealized example in which tunneling transitions are balanced by a single collective transition within the compact states. We have not at this point developed an associated phonon-coupled SU(N) model that exhibits this effect, but we expect that it will be possible to do so. More interesting is the question of whether such behavior will be present in more complicated phonon-coupled SU(N) models.

8.4. *Bursts*

The model described in the previous section leads has been studied in a companion paper,[50] and numerical results have been presented for the population evolution and the associated reaction rates. The reaction rates from that model can be reasonably approximated by

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[1]There has been interest in the connection between anomalies in metal deuterides and superradiance since very early in the field.[48,51]

$$\Gamma(t) \;=\; \frac{2N^2 V e^{-G}}{\pi\hbar} \; \mathrm{sech}\left(\frac{2NVe^{-G}}{\hbar}t\right) \tag{42}$$

This dynamical rate satisfies

$$N \;=\; \int_{-\infty}^{\infty} \Gamma(t)\; dt \tag{43}$$

It is reasonable to define a pulse time scale τ according to

$$\tau \;=\; \left[\frac{2NVe^{-G}}{\hbar}\right]^{-1} \tag{44}$$

We see that the product of the peak reaction rate with τ is proportional to N, so that we can form an estimate of N from

$$N \;=\; \pi\, \Gamma_{max}\tau \tag{45}$$

We can also express the coupling strength in terms of the rate and time scale according to

$$\frac{Ve^{-G}}{\hbar} \;=\; \frac{1}{2N\tau} \;=\; \frac{1}{2\pi\Gamma_{max}\tau^2} \tag{46}$$

If we consider a representative excess heat pulse with $\Gamma = 10^{12}$ sec^{-1} and $\tau = 5$ hours, and consider it to be due to a single coherent process of the kind under discussion, then obtain

$$\frac{Ve^{-G}}{\hbar} \;=\; \frac{1}{2\pi\Gamma_{max}\tau^2} \;=\; 5\times 10^{-22}\; \frac{\text{rad}}{\text{sec}}$$

If we assume that V is 10 MeV, then we obtain

$$e^{-G} \;=\; 3\times 10^{-44}$$

which is on the general order of the Gamow factor for molecular D_2.

8.5. *Connection with Experiment*

(1) We mentioned above that the observation of anomalies in all cases imply rates that are inconsistent with rates which would be predicted for incoherent processes involving tunneling. Tunneling as a coherent process with a superradiant enhancement leads to reaction rate estimates that are consistent with observations.

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(2) Most experimental results on anomalies in metal deuterides (including low-level dd-fusion, excess heat, and other effects) show a burst effect, in which the effect is absent, then turns on, then turns off again.[52] We propose that the burst effect is a consequence of superradiance. In the case of excess heat, the idealized burst model leads to a relation between the burn rate, the pulse length, and an associated Dicke number which may be on the order of the number of helium nuclei produced. Such a relation has not been verified experimentally, and may not be straightforward to verify, but may be worthy of study.

(3) In the limit that a single heat burst event is isolated, it may be possible to gain information about the tunneling factor for a metal deuteride.

(4) We have not yet addressed the issue of what phonon frequencies are involved yet. The requirement for the exchange of 20 or more phonons in order to stabilize the compact states produces a requirement on the energy density associated with phonon excitation, independent of frequency. However, phonon modes are lossy. The highest power densities reported for excess heat production are in the range of several kilowatts per cubic centimeter. We conclude therefore that the highest phonon frequencies likely to be involved are on the order of 1 GHz.

(5) There is no particular difference between the time-dependence of excess heat bursts and those associated with neutrons or charged particles. Our studies of the phonon-coupled SU(N) models so far suggest that the details of the coupling between the nuclei and phonons is such to result in similar mixing in the nuclear and phonon degrees of freedom, with similar numbers of phonons exchanged, reasonably independent of phonon frequency. However, if the phonon frequency is low, then there would not be much energy exchange in association with the phonon exchange. It may be that the primary difference between the different operating regimes may simply be due to which phonon frequencies are involved. If the nuclear energy is not converted to phononic energy, then the compact states could reform molecular states at the end of a pulse, and only a small fraction of the total be expressed as incoherent products during the process.

9. Conclusions

The most basic conclusion from the ideas and models presented here is that the new effects, although wildly at variance with what we know from nuclear physics in textbooks, may follow new physical laws that are reasonable, understandable, and amenable to analysis on the same footing as in other disciplines. The approach presented here provides a starting place from which the disparate anomlies might be understood systematically as consequences of an underlying physical picture.

A unifying picture of the anomalies is emerging from the ideas presented here. The need for high loading in the Fleischmann-Pons experiment is understood within the theory as a need for producing double occupancy. Vacancies, high loading and elevated temperature can all help in this regard. Current helps to achieve high loading, but within the theory it is also producing phononic excitation needed to couple nuclear reactions at different sites. Fast alpha emission within the model is perhaps the most direct signature of that reaction energy from one site can be expressed at another site. A consideration of the site-other-site mechanism in detail leads ultimately to the conclusion that there must be compact states, and

anomalous proton and alpha signals in the Kasagi experiment seem to provide evidence that the compact states are real. The stability of the compact states and the relative lack of two-body products from the three-deuteron interaction are interpreted as being indicative of the ability of the lattice to transfer large amounts of angular momentum to the microscopic nuclear system. Stable compact states are predicted to participate in a large number of site-to-site exchange reactions which help stabilize them and allow for energy exchange with the lattice, which is supported by experiments that show ^{4}He emission correlated with the excess energy with a Q value observed to be near 24 MeV. The enormous enhancement in the tunneling rate is seen within the model to be a signature of Dicke enhanced coherent tunneling, and the observed reaction rates and dynamics seem to be consistent with idealized models describing such transitions.

Research on anomalies in metal deuterides has from the beginning not been included as part of the mainstream scientific endeavor. There has not existed a program of systematic investigation into the different issues and aspects that we have been concerned with in this manuscript. Consequently, many of the important physical statements that might be made are not yet backed up by a solid body of experiment which might otherwise settle things. For example, we have no direct observations of deuterons in double occupancy in any of the relevant experiments. We have no clear demonstration of phonon exchange or angular momentum exchange in a fusion reaction in isolation. We do not have clean systematic spectra of alphas, protons and neutrons in connection with the site-other-site reaction mechanism discussed above, as can be found in the nuclear literature on photodisintegration. The experimental basis that supports the possible existence and properties of compact states as discussed above is not particularly strong.

There are many important related issues that we did not discuss in this manuscript. For example, the models do not obviously exclude similar processes in the case of the p+d system, which may be relevant to claims of anomalies in light water experiments. We have not discussed dephasing of the coherence present in the models. Our discussion has sought to retain a focus on basic physics issues, so we have not examined issues relating to the optimization of excess heat producing systems. There are experimental claims for other anomalies, such as the transmutation effect recently reported by Iwamura, which we have not considered.

It is our belief that continued work along these lines will lead to better models, and a generally agreed upon satisfactory understanding of the phenomena in general. We remain interested in the development of engineering models that will be useful for applications of the technology implied by the new physics.

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Appendix: Coupled-Channel Equations for the Two-Site Problem

The optimization of the lattice channel separation factors in this case leads to coupled-channel equations of the form

$$EA_n = E_1(n)A_n + \sum_{n'lm} \int_0^\infty v_{lm}^{nn'}(r)[P_{n'lm}^a(r) + P_{n'lm}^b(r)]dr \tag{47}$$

$$E\,P_{nlm}^a(r) = \left[E_2(n) - \frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V^a(r) \right] P_{nlm}^a(r)$$
$$+ \sum_{n'} [v_{lm}^{nn'}(r)]^* A_{n'} + \sum_{n'}\sum_{l'm'} \int_0^\infty v_{l'm'}^{nn'}(s)\,P_{n'lml'm'}^{ab}(r,s)\,ds \tag{48}$$

$$E\,P_{nlm}^b(s) = \left[E_3(n) - \frac{\hbar^2}{2\mu}\frac{d^2}{ds^2} + \frac{\hbar^2 l(l+1)}{2\mu s^2} + V^b(s) \right] P_{nlm}^b(s)$$
$$+ \sum_{n'} [v_{lm}^{nn'}(s)]^* A_{n'} + \sum_{n'}\sum_{l'm'} \int_0^\infty v_{l'm'}^{nn'}(r)\,P_{n'l'm'lm}^{ab}(r,s)\,dr \tag{49}$$

$$E\,P_{nlml'm'}^{ab}(r,s) = \left[E_4(n) - \frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V^a(r) - \frac{\hbar^2}{2\mu}\frac{d^2}{ds^2} \right.$$
$$\left. + \frac{\hbar^2 l'(l'+1)}{2\mu s^2} + V^b(s) \right] P_{nlml'm'}^{ab}(r,s) + \sum_{n'} [v_{l'm'}^{nn'}(s)]^* P_{n'lm}^a(r)$$
$$+ \sum_{n'} [v_{lm}^{nn'}(r)]^* P_{n'l'm'}^b(s) \tag{50}$$

where

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$$E_1(n) = 2E[^4\text{He}] + \hbar\omega_0\left(n + \frac{1}{2}\right)$$

$$E_2(n) = E_3(n) = E[^4\text{He}] + E[n] + E[^3\text{He}] + \hbar\omega_0\left(n + \frac{1}{2}\right)$$

$$E_4(n) = 2E[n] + 2E[^3\text{He}] + \hbar\omega_0\left(n + \frac{1}{2}\right)$$

We have studied equations similar to these, with the conclusion that they give rise to significant exchange effects as well as compact state solutions (which can be stable or unstable). The compact state energies are dependent on the strength of coupling, as well as the angular momentum transferred through phonon exchange.