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# A UNIFIED MODEL FOR ANOMALIES IN METAL DEUTERIDES

P. L. Hagelstein

Research Laboratory of Electronics, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, MA 02139

## ABSTRACT

Nuclear reactions in a lattice are described using an extension of the resonating group method to include the lattice explicitly. Phonon exchange during fusion and dissociation reactions is predicted Second-order site-other-site reactions are predicted under conditions where the reactions at each site exchange phonons with a common phonon mode. The null reaction in which a dd-fusion at one site is coupled to $^4$He dissociation at another site is modeled. Coupled-channel equations are developed for the two-site problem, as an illustration of the application of the lattice resonating group method. We have proposed previously that there should exist compact state solutions of the coupled-channel equations, as the associated exchange potential can be attractive. Such states have been proposed to account for the Kasagi effect, and to provide a foundation for many of the anomalies that are seen in metal deuterides. Our analysis of the two-site system suggests so far has not yielded compact state solutions. Preliminary results for the many-site problem are presented, which leads to evidence in support of the stability of the compact states, and which leads to a new overall picture for the anomalies.

## 1. INTRODUCTION

There have been a variety of anomalies claimed to have been observed in metal deuterides and in metal hydrides over the past 13 years. The principal effects that have been claimed include: temperature excess, energy production, heat with quantitative $^4$He, slow tritium production, low level *dd*-fusion, gamma emission, fast low-mass ion emission that is not from *dd*-fusion, induced radioactivity, massive transmutation, and the observation of reaction products from beam experiments consistent with a three-deuteron reaction. From our perspective, the most important theoretical problem to be addressed is one of mechanism. Most physicists would agree that the new effects claimed to have been observed are not consistent with vacuum nuclear physics as has been studied for the past 80 years. The point of view taken by the physics community in light of the experimental claims has been to question the competence of those performing the measurements. We chose instead to contemplate the theoretical implications of the experimental claims.

After considering a very large number of approaches to the theoretical problem, it appears that the most promising route for understanding, and hence modeling, the experimental claims is to replace the vacuum nuclear physics formulation with a new formulation that includes solid-state effects implicitly at the outset. While this may seem to be a very obvious starting place, the reader should be assured that this obviousness is entirely retrospective.

## 2. INCLUDING THE LATTICE IN THE PROBLEM FORMULATION

There are two basic formulations that have been used to describe fusion reactions in the literature: the resonating group method,[1] and the R-matrix method.[2] The extension of these methods to include solid state effects is completely straightforward, as we have discussed previously.[3] The resonating group method may be thought of as specifying an approximate multichannel variational wavefunction

$$\Psi = \sum_j \Phi_j F_j \tag{1}$$

in which the internal nuclear degrees of freedom are described by basis states $\Phi_j$, and the relative channel separation factors $F_j$ describe the physics associated with the separation of the center of mass of the reacting and product nuclei. The optimization of the channel separation factors leads to coupled-channel equations that we may write formally as

$$EF_i = \left\langle \Phi_i \left| \hat{H} \right| \Phi_i \right\rangle F_i + \sum_j \left\langle \Phi_i \left| \hat{H} - E \right| \Phi_j F_j \right\rangle \tag{2}$$

The generalization of the approach to include solid state effects involves the replacement of the channel separation factors $F_j$ with lattice channel separation factors $\Psi_j$ that include in principle a description of all of the center of mass coordinates in the solid on equal footing. The lattice resonating group method is then based on an approximate multichannel variational wavefunction

$$\Psi = \sum_j \Phi_j \Psi_j \tag{3}$$

The optimization of the associated lattice channel separation factors $\Psi_j$ leads to coupled lattice multichannel equations

$$E\Psi_i = \left\langle \Phi_i \left| \hat{H} \right| \Phi_i \right\rangle \Psi_i + \sum_j \left\langle \Phi_i \left| \hat{H} - E \right| \Phi_j \Psi_j \right\rangle \tag{4}$$

The R-matrix method can be extended similarly to the lattice case. Our focus here will be on the lattice resonating group method, as it is the simpler formulation to present basic concepts.

The basic claim is that the inclusion of the solid-state part of the problem at the outset is ultimately all that is needed in order to generalize vacuum nuclear physics to be relevant to developing models for the various anomalies. A seemingly innocuous physical statement is proposed, however, the ramifications are enormous.

## 3. PHONON EXCHANGE AND SECOND-ORDER SITE-OTHER-SITE REACTION

One would not expect that the exchange of a few phonons would have much impact on fusion rates or reaction channels of first-order reactions in the lattice. Perhaps the most promising route to demonstrate directly the existence of a phonon exchange effect is to seek a modification of the angular dependence of the reaction products for very low energy fusion reactions in a solid with a very strong uniform optical phonon field. This would involve careful low energy accelerator experiments in which the angular distribution would be measured with and without optical phonon excitation. A small change in the angular distribution of the dd-fusion products would occur if a strong phonon exchange effect were present. If measured, it would prove that angular momentum exchange between a phonon field and the microscopic nuclear system can occur. No such experiments have been done or are planned to the author's knowledge.

However, the new formulation allows for the possibility of a novel class of second-order reactions. A second-order reaction is possible for reacting nuclei at two different sites as long as phonon exchange occurs with a common phonon mode.[4] The most important of such a second-order reaction in a metal deuteride is the null reaction

$$\left(d + d\right)_a + \left(^4He\right) \leftrightarrow \left(^4He\right)_a + \left(d + d\right)_b \tag{5}$$

Two deuterons fuse at one site, and a helium nucleus dissociates at another site, the two processes being coupled together through phonon exchange with a common phonon field. The microscopic selection rules require an E2 electric quadrupole interaction, which in this case comes about through phonon exchange. This reaction we will discuss further below.

This basic mechanism also implies other second-order reactions. Relevant to light water reactions is the $^3$He version of the null reaction

$$\left(p+d\right)_a+\left(^3He\right)\leftrightarrow\left(^3He\right)_a+\left(p+d\right)_b \tag{6}$$

The energy from a fusion reaction at one site can disintegrate a nucleus at another state, through a second-order reaction of the form

$$\left(d+d\right)_a+\left(^A Pd\right)\rightarrow\left(^4He\right)_a+\left(^{A-4}Ru+\alpha\right)_b \tag{7}$$

In this case, the alpha particles would be ejected at energies between 18-21 MeV, as reported by Chambers.[5] The observations of Cecil in $TiD_2$ can be accounted through a similar mechanism.[6] Iwamura has recently claimed the observation of substantial transmutation effects.[7] The specific cases that he reports, assuming that the effect is real, could be accounted for by site-other-site reactions of the form

$$\left(d+d\right)_a+\left(^A Z\right)\rightarrow\left(^4He\right)_a+\left(^{A-12}\left(Z-6\right)+^{12}C\right)_b \tag{8}$$

assuming that the energetic $^{12}$C nucleus produced as a result subsequently reacts with a nearby nucleus in a $^{12}$C ($^{A'}$Z',$^{A'+8}$[Z'+4]) $^4$He reaction.

## 4. TWO-SITE MODEL WITH A WIGNER INTERACTION

As in our previous work, we seek the simplest models that contain the physics of interest in order to illustrate the effects under discussion. In the many-body problem of interest, there are a very large number of sites that can interact. Here we restrict ourselves to only two active sites. Many phonon modes in general are involved. Here we reduce the problem down to a single highly excited mode, while all other modes are accounted for in local coordinates.[8] The nuclear interaction depends on spin and isospin in a complicated way. Here we propose to simply use a scalar Wigner Gaussian interaction. In the end, the resulting Hamiltonian for the coupled lattice and nuclear system is of the form

$$\hat{H}=-\sum_j\frac{\hbar^2\nabla_j^2}{2M_j}-\sum_{i<j}V_0e^{-\alpha\left|\boldsymbol{R}_i-\boldsymbol{R}_j\right|^2}+\sum_{i<j}\frac{e^2}{\left|\boldsymbol{R}_i-\boldsymbol{R}_j\right|}-\frac{\hbar^2}{2\mu}\frac{d^2}{dq^2}+V\left(q\right)+V_{loc} \tag{9}$$

The sum over nuclear coordinate ranges over four nucleons at one site, and four more nucleons at a second site. Nucleons interact with each other through an attractive scalar Gaussian interaction and Coulomb interaction. The highly excited phonon mode has amplitude $q$. For the two sites to interact with a common phonon mode, the two sites must be close together, within several hundred Angstroms to a micron, depending on the phonon mode in question. The optical phonon modes between 8 and 15 THz in PdD would probably be most effective. However, the highest acoustical phonon modes in the THz region may show a response, and one might expect the strong coupling between electrons and phonons to lead to a response at higher frequencies. The local potential seen by either a pair of deuterons or a helium nucleus at each site is presumed to be approximately spherical in the absence of effects due to the highly excited phonon mode. The nuclear and Coulomb interaction depends on the highly excited phonon mode through the relative deuteron center of mass coordinate of the deuterons.

An approximate wavefunction for the coupled lattice and nuclear system is developed according to

$$\Psi=\sum_n A_n\left|\Phi_{He}^a\Phi_{He}^b\phi_n\right\rangle+\sum_{nlm}\left|\Phi_{dd}^a\Phi_{He}^b\phi_nY_{lm}^a\right\rangle\frac{P_{nlm}^a\left(r\right)}{r}+\sum_{nlm}\left|\Phi_{He}^a\Phi_{dd}^b\phi_nY_{lm}^b\right\rangle\frac{P_{nlm}^b\left(s\right)}{s}$$

$$+\sum_n\sum_{lm}\sum_{l'm'}\left|\Phi_{dd}^a\Phi_{dd}^b\phi_nY_{lm}^aY_{l'm'}^b\right\rangle\frac{P_{nlml'm'}^{ab}\left(r,s\right)}{rs} \tag{10}$$

We consider in this model that the terms $\left|\cdots\right\rangle$ are to be taken as basis functions, and the various *P* functions are the residual radial lattice coupled-channel separation factors. The basis functions include internal nuclear $\Phi$ functions, that keep track of whether the two sites, *a* and *b*, are occupied by a deuteron pair or a helium nucleus. The highly excited phonon mode is accounted for by $\phi_n$. The angular momentum associated with the local radial channel separation factor is accounted for by the various spherical harmonics $Y_{lm}$.

The optimization of the wavefunction leads to lattice coupled-channel equations of the form described previously. For example, the two-helium channel is optimized to give

$$EA_n = \left\langle \Phi^a_{He}\Phi^b_{He}\phi_n \left| \hat{H} \right| \Phi^a_{He}\Phi^b_{He}\phi_n \right\rangle A_n + \sum_{n'lm} \left\langle \Phi^a_{He}\Phi^b_{dd}\phi_n \left| \hat{H} - E \right| \Phi^a_{dd}\Phi^b_{He}\phi_{n'} Y^a_{lm} \frac{P^a_{n'lm}(r)}{r} \right\rangle$$
$$+ \sum_{n'lm} \left\langle \Phi^a_{He}\Phi^b_{He}\phi_n \left| \hat{H} - E \right| \Phi^a_{He}\Phi^b_{dd}\phi_{n'} Y^a_{lm} Y^b_{lm} \frac{P^b_{n'lm}(s)}{s} \right\rangle \tag{11}$$

This equation and equivalent equations for other channels are reduced to radial coupled-channel equations of the form

$$EA_n = \left[ 2E_{He} + \hbar\omega_0 \left( n + \frac{1}{2} \right) \right] A_n + \sum_{n'lm} \int_0^\infty v^{nn'}_{lm}(r) \left[ P^a_{n'lm}(r) + P^b_{n'lm}(r) \right] dr \tag{12}$$

$$EP^a_{nlm}(r) = \left[ E_{He} + E_{dd} + \hbar\omega_0 \left( n + \frac{1}{2} \right) - \frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V^a(r) \right] P^a_{nlm}(r)$$
$$+ \sum_{n'} \left[ v^{nn'}_{lm}(r) \right]^* A_{n'} + \sum_{n'} \sum_{l'm'} \int_0^\infty v^{nn'}_{l'm'}(s) P^{ab}_{n'lml'm'}(r,s)\, ds \tag{13}$$

$$EP^b_{nlm}(s) = \left[ E_{He} + E_{dd} + \hbar\omega_0 \left( n + \frac{1}{2} \right) - \frac{\hbar^2}{2\mu}\frac{d^2}{ds^2} + \frac{\hbar^2 l(l+1)}{2\mu s^2} + V^b(s) \right] P^b_{nlm}(s)$$
$$+ \sum_{n'} \left[ v^{nn'}_{lm}(s) \right]^* A_{n'} + \sum_{n'} \sum_{l'm'} \int_0^\infty v^{nn'}_{l'm'}(r) P^{ab}_{n'l'm'lm}(r,s)\, dr \tag{14}$$

$$EP^{ab}_{nlml'm'}(r,s) = \left[ 2E_{dd} + \hbar\omega_0 \left( n + \frac{1}{2} \right) - \frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V^a(r) - \frac{\hbar^2}{2\mu}\frac{d^2}{ds^2} \right.$$
$$\left. + \frac{\hbar^2 l'(l'+1)}{2\mu s^2} + V^b(s) \right] P^{ab}_{nlml'm'}(r,s) + \sum_{n'} \left[ v^{nn'}_{l'm'}(s) \right]^* P^a_{n'lm}(r) + \sum_{n'} \left[ v^{nn'}_{lm}(r) \right]^* P^b_{n'l'm'}(s) \tag{15}$$

These equations are derived assuming a harmonic oscillator model for the highly excited phonon mode.

## 5. PHONON EXCHANGE

Phonon exchange appears naturally within the model. We have pursued a calculation of phonon exchange in the case of Gaussian nuclear wavefunctions.

$$\Phi_d = \Phi_2 = N_2 e^{-\beta_2 |\boldsymbol{r}_1 - \boldsymbol{r}_2|^2} \tag{16}$$

$$\Phi_{He} = \Phi_4 = N_4 e^{-\beta_4 |\boldsymbol{r}_1 - \boldsymbol{r}_2|^2} e^{-\beta_4 |\boldsymbol{r}_1 - \boldsymbol{r}_3|^2} e^{-\beta_4 |\boldsymbol{r}_1 - \boldsymbol{r}_4|^2} e^{-\beta_4 |\boldsymbol{r}_2 - \boldsymbol{r}_3|^2} e^{-\beta_4 |\boldsymbol{r}_2 - \boldsymbol{r}_4|^2} e^{-\beta_4 |\boldsymbol{r}_3 - \boldsymbol{r}_4|^2} \tag{17}$$

The overlap integral between a deuteron pair and a helium nucleus depends on the relative distance between the deuteron center of mass coordinates. If we naively replace *H-E* by the scalar Wigner interaction, then we obtain

$$\begin{aligned} \left\langle \Phi_{dd} \left| \hat{H} - E \right| \Phi_{He} \right\rangle = -V_0 N_2^2 N_4 \int d^3 \boldsymbol{x}_{21} \int d^3 \boldsymbol{x}_{43} e^{-\beta_2 |\boldsymbol{x}_{21}|^2} e^{-\beta_2 |\boldsymbol{x}_{43}|^2} \\ \left[ e^{-\alpha |\boldsymbol{r}_1 - \boldsymbol{r}_3|^2} + e^{-\alpha |\boldsymbol{r}_1 - \boldsymbol{r}_4|^2} + e^{-\alpha |\boldsymbol{r}_2 - \boldsymbol{r}_3|^2} + e^{-\alpha |\boldsymbol{r}_2 - \boldsymbol{r}_4|^2} \right] \\ e^{-\beta_4 |\boldsymbol{x}_{21}|^2} e^{-\beta_4 |\boldsymbol{r}_1 - \boldsymbol{r}_3|^2} e^{-\beta_4 |\boldsymbol{r}_1 - \boldsymbol{r}_4|^2} e^{-\beta_4 |\boldsymbol{r}_2 - \boldsymbol{r}_3|^2} e^{-\beta_4 |\boldsymbol{r}_2 - \boldsymbol{r}_4|^2} e^{-\beta_4 |\boldsymbol{x}_{43}|^2} \end{aligned} \tag{18}$$

Where $\boldsymbol{x}_{21} = \boldsymbol{r}_2 - \boldsymbol{r}_1$ and $\boldsymbol{x}_{43} = \boldsymbol{r}_4 - \boldsymbol{r}_3$. The distance between the two-deuteron center of mass coordinates is a function of the amplitude of the highly excited phonon mode

$$\frac{1}{2}\left(\boldsymbol{r}_3 + \boldsymbol{r}_4\right) - \frac{1}{2}\left(\boldsymbol{r}_1 + \boldsymbol{r}_2\right) = \bar{\boldsymbol{r}} + \Delta \boldsymbol{u} \hat{q} \tag{19}$$

Here $\bar{\boldsymbol{r}}$ is the residual radial separation coordinate, and $\Delta \boldsymbol{u} \hat{q}$ describes the relative motion due to the highly excited phonon mode. The basic picture that underlies this discussion is one in which two deuterons occupy a single site, either due to high loading, high temperature, or due to the presence of vacancies within the metal deuteride. Occasionally, the deuterons tunnel close together. While close together, the deuterons are still part of the lattice, and constitute a component of the phonon modes of the lattice. When they are close together, the very strong nuclear and Coulomb interactions dominate over the interactions with relatively distant atoms that may be a few Angstroms away. However, the deuterons will still exhibit a response in the presence of strong phononic excitation, although a weak one, which must be computed using a linearization scheme that takes into account the very strong interactions the deuterons undergo while close together. The resulting relative motion that is accounted from the $\Delta \boldsymbol{u} \hat{q}$ term is expected to be on the order of fermis.

After much algebra and the use of the WKB approximation, we obtain for an interaction

$$\begin{aligned} \left\langle \Phi_{dd} \phi_n Y_{lm} \left| \hat{H} - E \right| \phi_{He} \phi_{n'} \right\rangle = -4V_0 \left[ \frac{8^{\frac{1}{4}} \left(2\beta_2\right)^{\frac{3}{2}} \left(4\beta_4\right)^{\frac{9}{4}}}{\pi^{\frac{1}{4}} \left(\beta_2 + 2\beta_4\right)^{\frac{3}{2}} \left(\beta_2 + 2\beta_4 + \frac{\alpha}{2}\right)^{\frac{3}{2}}} \right] e^{-K|\bar{\boldsymbol{r}}|^2} \sqrt{2l+1} \delta_{m,0} \\ \times \frac{1}{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} e^{-K|\Delta \boldsymbol{u}|^2 q_{\max}^2 \sin^2 \xi} i_l \left(2K\bar{r} \left|\Delta \boldsymbol{u}\right| q_{max} \sin \xi\right) \cos\left(\Delta n \xi\right) d\xi \end{aligned} \tag{20}$$

where $\Delta n$ is the number of phonons exchanged, and where

$$K\left(\alpha, \beta_2, \beta_4\right) = \frac{8\beta_4^2 + 4\beta_2\beta_4 + 4\beta_4\alpha + \beta_2\alpha}{\beta_2 + 2\beta_4 + \frac{\alpha}{2}} \tag{21}$$

$$i_n(z) = \sqrt{\frac{\pi}{2z}} I_{n+\frac{1}{2}}(z) \tag{22}$$

Our calculations so far indicate that a maximum local relative motion $|\Delta \boldsymbol{u}| q_{\max}$ on the order of half a fermi is sufficient to generate a significant two-phonon exchange interaction. Relative motion on the order of several fermis can result in the exchange of on the order of 10 phonons within this kind of model.

## 6. THE MANY-SITE PROBLEM

We have considered the generalization of the problem to the case of many sites. The mechanics of the construction of the many-site coupled channel equations are straightforward, however, the problem seems to be qualitatively richer as we discuss below. In conducting the study, we had hoped to obtain a continuum of compact state solutions, along the lines that we outlined in a recent lengthy review of the problem.[9] Our recent results suggest that the conclusions in this review are somewhat naïve, and that the basic picture requires some revision.

The many-site coupled-channel equations are of the basic form

$$EP_M^\beta = H_\beta P_M^\beta + \sum_{\alpha,k} v_k P_{M-1}^\alpha + \sum_{\gamma,k} < v_k \ | P_{M+1}^\gamma > \tag{23}$$

where $P_M^\beta$ is a many-site channel separation factor with configuration $\beta$ and with index *M* defined by

$$M = \frac{N_{dd} - N_{He}}{2} \tag{24}$$

There are a very large number of channels, and it quickly becomes impractical to attempt a direction solution of them. In our previous work, we made use of infinite-order Brillouin-Wigner perturbation theory in order to get some insight as to possible nature of the solutions. Here, we simply note that it appears that such an approach is simply not up to the problem when the coupling becomes strong enough to be interesting in terms of accounting for the experimental results. Instead, we must make use of alternate approximations.

Of fundamental concern is the question of whether there exist localized solutions to the many-site version of the coupled-channel equations. It seems *a priori* unlikely that an answer would be forthcoming without a brute force computation on the coupled-channel equations. Our efforts to date on this problem have so far not produced insight. For the purposes of the present discussion, we might adopt as an ansatz the assumption that we can define useful localized states which may or may not be stable, and proceed with the calculation in order to ascertain the goodness of the ansatz with solutions in hand. This appears to be a productive approach.

We propose to simplify matters further in order to allow us to make progress on the development of this very hard problem by assuming that all sites are identical, and furthermore, that the establishment of a localized state at each of these sites will involve the same local superposition of orbitals within the different angular momentum channels. These simplifications lead ultimately to a an approximate time-independent eigenvalue equation based on a Hamiltonian of the form

$$H = \Delta E(\Sigma_z + S) + \hbar\omega\left(n + \frac{1}{2}\right) + < h > (\Sigma_z + S) + \sum_{n'} (\Sigma_+ + \Sigma_-) V_{nn'} \delta_{nn'} \tag{25}$$

In this Hamiltonian the $\Sigma$ operators are pseudospin operators that are developed as a superposition over Pauli matrices at the different sites

$$\Sigma = \sum_i \sigma_i \tag{26}$$

The parameter *S* is the Dicke number for the system

$$S = \frac{N_{dd} + N_{He}}{2} \tag{27}$$

The localization energy for a single site is <*h*>, and the $V_{nn'}$ terms are integrals of the interaction potentials and localized orbitals summed over the different angular momentum channels.

We have encountered such a Hamiltonian previously, before we had considered the possibility of localized two-deuteron states, as perhaps applying to a many-body version of the problem in which molecular states would make phonon-mediated transitions to helium states. In that case, the hope was that the number of sites involved would be sufficiently large that the Dicke enhancement could offset the Gamow factors. Here, we apply the Hamiltonian now to the situation where compact states are making transitions, in which case there is no Gamow factor, and the coupling is very strong. In our previous work, we studied this kind of model in order to understand under what conditions such a model might lead to extended states that were sufficiently broad in *n* so as to allow coherence between the states with different number of fusion events and vastly different phonon number such that approximate energy conservation occurred. We were astonished at how this model stubbornly insisted on producing localized states in which the number of phonons exchanged was on the order of the associated dimensionless coupling constant. This being said, we are aware that the eigenfunctions of this Hamiltonian are generally not overly interesting in regards to relating to the physical problem in question, without further input to the problem.

## 7. INCLUDING LOSS

The basic problem with the model Dicke Hamiltonian lies in its high degree of symmetry when *n* and *S* are large, and *M* is small. In order to develop delocalized solutions, the symmetry needs to be broken somehow. Either we require coupling coefficients that depend strongly on *n* or *M*, or else we need some kind of additional potential that is highly nonlinear in one or both of these quantum numbers. It is the case that working in the limit where the number of helium nuclei that interact is on the order of the dimensionless coupling strength makes a difference with respect to delocalizing the solutions in *n* and *M* space.

There is another effect which is much more important, and which has a very strong dependence on *M*. This includes loss terms. For example, when two deuterons fuse in the many-site problem, the off-resonant energy $\Delta E$ (24 MeV) is more than enough to fuel recoil between localized deuterons and many other highly energetic decay modes. The presence of such decay modes completely destroys the underlying symmetry of the problem, and produces significant delocalization of the wavefunction in *n* and *M* space. Unfortunately, the inclusion of decay channels into a Hamiltonian is not particularly straightforward. Such problems in other disciplines are often handled using density matrices. We wish not to adopt such a formulation here, as the associated complications would likely make further progress more difficult due to the added complexity of the approach.

Instead, we prefer to think about the problem as a probability flow problem, as we will outline below. In order to derive the relevant flow problem, we consider a Hamiltonian of the form

$$H = H_0 + V \tag{28}$$

We imagine that the problem divides up into three sets of basis states, source states, sink states, and states intermediate between the two. For example, we might consider deuteron pairs locally in molecular states to be part of the source states. States that contain energetic reaction products that result from recoil processes or other reactions are sink states. Intermediate states are those including helium nuclei or two-deuteron compact states in the sites of interest. We may divide the associated Hilbert space into three sectors that correspond to source basis states, sink basis states, and intermediate basis states. After all, loss can be thought of as simply transitions from a sector of Hilbert space that one is interested in, to other sectors. We can accomplish this splitting of the different sectors by taking advantage of Feshbach projection operators

$$P_i = \sum_j |\, \Phi_j >< \Phi_j \,| \tag{29}$$

where the summation *j* is over the basis states in sector *i*. The time independent Schrodinger equation for this Hamiltonian is

$$E\Psi = H_0\Psi + V\Psi \tag{30}$$

To split this equation into sector-dependent equations, we assume that the eigenfunctions contains components in the three different sectors

$$\Psi = \Psi_1 + \Psi_2 + \Psi_3 \tag{31}$$

The time-independent Schrodinger equation is then divided into sector-dependent equations given by

$$E\Psi_1 = H_1\Psi_1 + V_{12}\Psi_2 \tag{32}$$

$$E\Psi_2 = H_2\Psi_2 + V_{21}\Psi_1 + V_{23}\Psi_3 \tag{33}$$

$$E\Psi_3 = H_3\Psi_3 + V_{32}\Psi_2 \tag{34}$$

We identify $\Psi_1$ with the source sector, $\Psi_2$ with the intermediate states, and $\Psi_3$ with the sink states. In writing these equations, we presume that there is no direct coupling between source and sink states. The sink states can be eliminated as in infinite-order Brillouin-Wigner theory

$$\Psi_3 = \left[E - H_3\right]^{-1} V_{32}\Psi_2 \tag{35}$$

The intermediate sector equation then becomes

$$E\Psi_2 = H_2\Psi_2 + V_{21}\Psi_1 + V_{23}\left[E - H_3\right]^{-1} V_{32}\Psi_2 \tag{36}$$

The interaction between the intermediate sector and the sink sector appears in this equation in the same way as in infinite-order Brillouin-Wigner theory. When the resolvant operator has a pole in a continuum at energy *E*, then the inverse operator develops an imaginary component that describes decay. We see in this equation a description of the intermediate sector, driven by the source sector, and decaying to the sink sector. We can solve formally for the intermediate sector component of the wavefunction to obtain

$$\Psi_2 = \left[\, E - H_2 - V_{23}\left[E - H_3\right]^{-1} V_{32} \,\right]^{-1} V_{21}\Psi_1 \tag{37}$$

This accomplishes the development of a probability amplitude flow equation, complete with source and with sink. Although the underlying formulation is rigorously Hermitian throughout, the inverse operator describing the intermediate sector evolution is non-Hermitian with respect to the intermediate sector. We have included loss into a Schrodinger formulation in a useful way. We define the operator $K_2$ to be the intermediate sector Hamiltonian augmented with loss terms that are non-Hermitian with respect to the sector 2 basis states

$$K_2 = H_2 + V_{23}\left[E - H_3\right]^{-1} V_{32} \tag{38}$$

The intermediate state solution written in terms of this operator becomes

$$\Psi_2 = \left[E - K_2\right]^{-1} V_{21}\Psi_1 \tag{39}$$

This is interesting, as $K_2$ has eigenfunctions that are delocalized due to the presence of loss terms that are very nonlinear in $M$.

## 7. INTERMEDIATE STATE DISTRIBUTIONS

We have put together a computer code to analyze the intermediate state solutions along the lines outlined above. Let us consider a few examples in order to illustrate some of the systematics. In Figure 1, we show the logarithm of the probability distribution under conditions

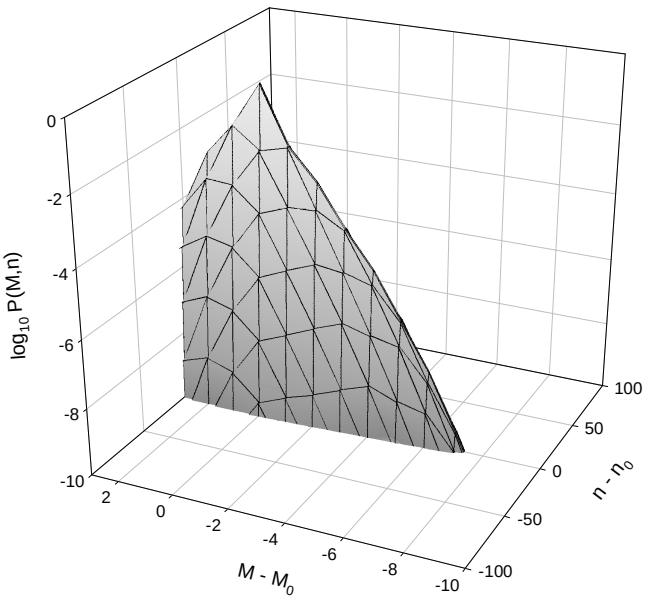


**Figure 1:** Probability distribution in the vicinity of the source in the case of weak coupling.

where the source is localized at ( $M_0$, $n_0$ ), and the coupling is weak. In this case, the initial condition corresponds to 3 helium atoms and 10 deuteron pairs. We see that the associated probability density is closely centered around the source, that the distribution is localized in phonon number, and that there is a spread in $M$ that is perhaps larger than one might expect. In the direction of negative $M$-$M_0$, which corresponds to more helium nuclei present, the states are very unstable, and the probability distribution decays moderately. The balance between the coupling strength and the decay rate determines the slope. In the other direction, we quickly reach the boundary at which all of the helium nuclei have dissociated, where there is a wall. These states are stable, as they are in serious energy deficit. Such a distribution corresponds to a low or modest level of conventional dd-fusion events, as well as some events in which the fusion energy is transferred to other decay modes within the lattice.

In Figure 2, we illustrate the same situation, except that the phonon oscillation amplitude is larger, and the interaction strength for phonon exchange is greater. We see that the stronger coupling leads to a much larger spread in $n$, which is a hallmark of this kind of model. The spread in $M$ is very significant as well, more so than in the previous example. This spread would like to be even larger, however, in both the positive and negative directions, the distribution hits walls as the number of helium nuclei and deuteron pairs is limited. We see that there is some avoidance of high loss regions of the configuration space, but that this is not a dominant effect in this problem.

In Figure 3, we present the logarithm of the probability distribution in the case where there are more helium nuclei present, and the losses are lower (corresponding to the development of higher angular momentum states). We see that the spread in phonon number is now much greater. We see another effect that is of great interest as well. We see that the probability distribution is strongly skewed into the region in

which $M$-$M_0$ is positive, avoiding the region in which $M$-$M_0$ is negative. The avoided region is where deuterons have fused to helium, and where the system has more energy than the local basis state energy, and hence where many decay processes are allowed. The probability distribution is seen to be favoring low-loss regimes, and hence minimizing the overall loss. This is very interesting, and appears to be a fundamental characteristic of this quantum system.

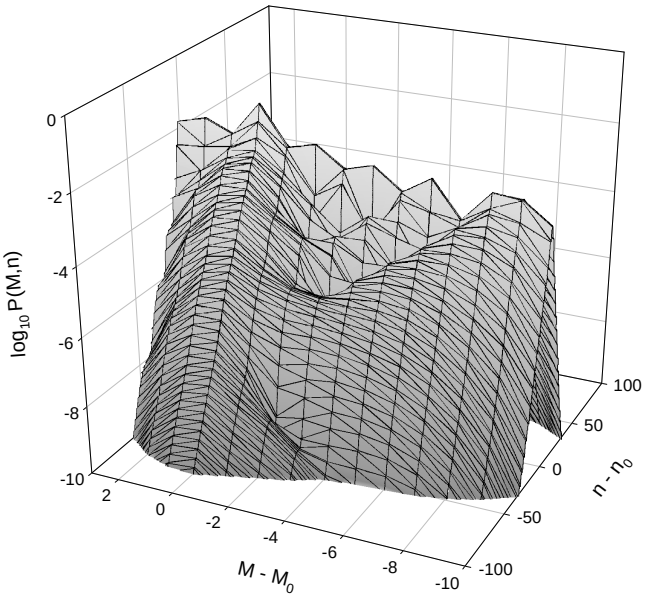


**Figure 2:** Probability distribution in the vicinity of the source in the case of moderate coupling.

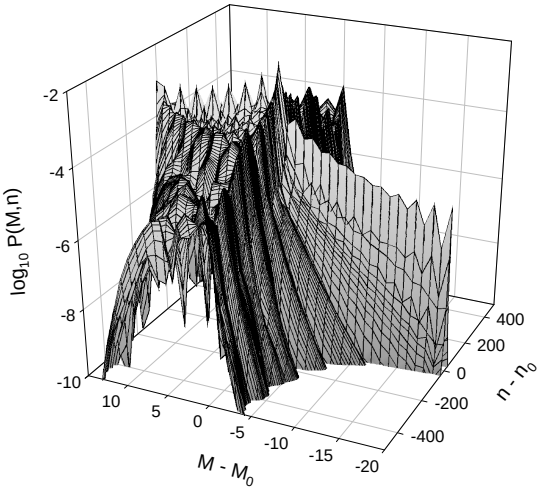


**Figure 3:** Probability distribution in the vicinity of the source in the case of strong coupling. Only a restricted range in $n$-$n_0$ has been included in the plot.

The spread of the distribution in phonon number increases as the strength of the coupling, and decreases under conditions in which the loss is large. It is possible to develop some intuition from these results as to how this problem works. The part of the Hamiltonian that describes fusion and dissociation transitions in this context serves as a kind of kinetic energy operator for the problem. The solutions appear to be outwardly oscillatory away from the source. As long as the probability amplitude avoids lossy regions,

then there appears to be a flow from the source into the positive $M$-$M_0$ corridor, confined on one side by a wall, and on the other side by an impedance mismatch associated with a high loss region. This flow is increased by a stronger coupling between the states, and inhibited only by the boundary loss. Our calculations so far have indicated that the transport of probability amplitude through the corridor can easily extend for more than a thousand quantum numbers in $n$-$n_0$. Altogether this is indicative of a rather efficient mechanism for coupling excitation and energy between the nuclear and phonon degrees of freedom.

## 8. STABILITY OF THE COMPACT STATES

The formulation and results given above allow us to re-examine the question of the stability of the compact states in light of the solutions that we have obtained. Stability can be assessed from two different points of view. On the one hand, we may look at the average loss rate for the intermediate probability distribution, and judge the stability of the compact states based on the resulting decay rate per site. We discussed above that most of the probability distribution is in the low-loss regime corresponding to the system being in relative energy deficit, in which the channels through which the compact states might separate by recoil are closed. Loss numbers estimated based on the presumption that recoil occurs freely wherever energetically allowed show that the stability improves dramatically as a function of the ability of the distribution in $M$ and $n$ to localize in regions of stability. We have seen up to three orders of magnitude improvement in the decay rate as measured in this way.

On the other hand, we might look at the stability of the compact states as measured by whether the exchange terms lead to a net positive or negative energy contribution as measured by

$$< V >= \left\langle \Psi_2 \left| \sum_{n'} \left( \Sigma_+ + \Sigma_- \right) V_{nn'} \delta_{nn'} \right| \Psi_2 \right\rangle \tag{40}$$

This interaction energy is negative under most conditions, which corresponds to the local exchange interaction being attractive. This argues in support of the compact states being localized. The corresponding local exchange energy that we have seen in the calculations done so far has approached 1 MeV. This argument needs to be developed further, but these results support the premise that stable compact states exist in the case of the many-site problem. It remains to establish precisely the conditions under which they are stable, however, the present results is indicative that only a relatively small number of sites are required for this to be so. Such a result is consistent with what we found when considering the two-site problem.

## 9. THE OVERALL PICTURE

The new results that we have described in this work leads to an overall picture that is somewhat different from that discussed earlier this year.[9] In the old picture, compact states could be developed at a continuum of energies ranging from the molecular state energy to the helium ground state energy. According to the present results, the compact states locally will have a significant localization energy which can be on the order of an MeV, and in addition a negative exchange energy that will produce a continuum of state energies which can extend down to the molecular state energy and below. It does not appear likely that the compact state energy distribution will extend down anywhere close to the helium state energy. There is no real reason for this to be the case, and our proposal that it might the case was clearly naïve.

Otherwise, the new overall picture is very much like what we described previously. Weak coupling leads to compact states with low angular momentum that are highly unstable against fusion reactions. Strong coupling with more than 10 sites with helium occupation interacting with a highly excited phonon mode begins to allow for the development of significant probability in states that are stabilized by virtue of energy deficiency. The associated loss modes include fusion reactions, simple deuteron-deuteron recoil, and the transfer of excitation to loss modes at other sites (such as alpha ejection and other low mass disintegration modes). Very strong coupling that involves large amplitude of local phonon-induced relative motion leads to high angular momentum compact states with very good associated stability, and this allows for the development of extremely large spread in $n$. In this regime, one might expect a large scale conversion of compact deuteron pairs to helium with the reaction energy expressed as an increase in the phonon number of the highly excited phonon mode.

A high level macroscopic picture of the system might be proposed based on the models described above. Deuterium is loaded into a metal host through any one of a variety of methods. The ideal metal host maximizes the local molecular state concentration, which can be accomplished through a combination of high loading, the creation of a large number of host metal atom vacancies, and through heating in the case that the molecular state energy is more than a few kT. Transitions to compact states are mediated through the presence of very strong excitation of an optical phonon mode, or any relevant hybrid electron-phonon mixed mode, such that deuterons are moved toward and away from each other when they are very close on a nuclear scale (albeit by a very small amount). To achieve high optical phonon excitation might be done in any number of ways. In many experiments, deuterium is fluxed through the metal deuteride. We have proposed previously that when deuterons transport down a sudden chemical potential barrier, that efficient optical phonon generation will result when the barrier is more than about 50 meV. Such differences in the local chemical potential are present between different crystallites within a homogeneous metal deuteride. Fluxing deuterons through a metal bilayer is expected to generate optical phonons even more efficiently, and experiments based on this method appear to give very interesting results. Precisely what physical phenomena are expressed depends on a variety of details, such as the level of optical phonon excitation, how many molecular states are occupied within an optical phonon mode, as well as how many helium nuclei are situated in useful sites – most or all of which are presently uncontrolled experimental variables.

The basic picture also applies to the $^3$He reaction branch, in which proton deuteron molecules and compact states dominate the new physics. There is presently no experimental evidence in support of a proton deuteron compact state analog of the Kasagi state. One would hope that this problem might be addressed. Heat production in mixed proton and deuteron systems should be accompanied by the production of $^3$He through the mechanisms indicated. To date, no evidence has been developed in support of the presence of $^3$He in association with light water experiments. Due to the absence of strong-force mediated fusion pathways for the proton-deuteron reaction, the stability of the compact states is much improved relative to the two-deuteron system. The models discussed here should apply with appropriate modifications to the proton-deuteron problem, and based on what we might surmise based on the discussions above, the proton deuteron system should be much more favorable in terms of the generation of compact states, the stability of them, and the possibility of making heat and inducing dissociation in neighboring atoms with low dissociation energies. Given the lower reaction energy, and the absence of strong-force fusion channels, the proton-deuteron system will likely be harder to diagnose. Experimental demonstrations of mechanisms will be more challenging in general.

## 10. DISCUSSION

Our discussion above has focused on the generalization of the resonating group method from the vacuum case to include the lattice. Within this formulation phonon exchange occurs during a nuclear reaction, which has little impact on first-order reactions. New second-order site-other-site reactions are predicted within this formulation. During the past several years, we have studied various models for two-site interactions and also for many-site interactions. The null reaction in which the fusion of a deuteron pair at one site is coupled to the dissociation of a helium nucleus at another site is clearly the most important such reaction in metal deuterides. We concluded some time ago that when the helium nucleus dissociates to form a deuteron pair, the deuteron pair introduced in close proximity has difficulty separating. The same Coulomb barrier that makes tunneling together from atomic distances difficult also inhibits the tunneling apart of two deuterons that happen to have been created within fermis of one another. This argument would suggest that new two-deuteron compact states should form within the model.

We have commented previously that the compact states within the model may be observable in accelerator experiments. We have proposed that the Kasagi effect[10] (apparent three-body ddd-fusion) may be due to a fast incident deuteron striking a deuteron pair in a compact state

$$d + \left(d + d\right)_{compact} \rightarrow p + n + \alpha \qquad (41)$$

Stable compact states would have a high angular momentum. The presence of a high two-body angular momentum would inhibit the two-body exit channels.[4]

The many-body model that results appears to describe a complicated situation. Deuteron pairs in molecular states within the metal can make transitions to compact states in a “slow” version of the null

reaction, but only when a strong component of optical phonon excitation is present. Null reaction transitions between compact two deuteron states are very fast. In the limit that only a few phonons are exchanged in each interaction, the compact states produced are unstable against the normal dd-fusion reactions (leading to $p+t$ and n+$^3$He). In this case, only compact states with energy near the molecular state energy are occupied, and dd-fusion reaction products would be observed. In this case also, a fusion reaction at one site can couple to a disintegration event at another site, leading to alpha ejection and the emission of other low mass ions. In the $p+d$ version of the model, the compact proton-deuteron states are much more stable. Nevertheless, there are many other-site disintegration paths available to take up the energy for a compact $p + d \rightarrow {}^3He$ fusion at one site.

When the local relative motion between deuterons becomes large (on the order of several fermis), then many phonons can be exchanged, and the accessible compact states are stabilized against conventional fusion reaction pathways (by the centripetal potential barrier). This should allow for a large quantum spread of the mixed states in phonon number, in which case pathways open for tritium production, or helium production if the spread is even greater.

We have focused on the simple two-site model in order to illustrate the basics of what is required of a model in order to show the effects under discussion. We have succeeded in outlining how phonon exchange works within the framework of a simple scalar nuclear interaction model. The two-site model does not appear to lead to compact two-deuteron states, based on the solutions that we have obtained so far. The reason seems to be that the coupling in the case of two sites is just too weak.

We have recently formulated the many-site version of the problem. It is clear from the discussion given above that the current version of the many-site problem is much richer than what we speculated about previously. We have made a connection between the underlying coupled-channel problem of the lattice resonating group method, and a many-site Dicke Hamiltonian similar to what we proposed previously before we became aware of the possible existence of two-deuteron compact states. We have formulated the intermediate state problem as a Schrodinger picture flow problem between different sectors in Hilbert space. An initial set of models that implement the flow problem have been implemented, and the results begin to illustrate how things work within the model. The inclusion of loss within the flow problem is a critical component of the problem. The probability distribution in the intermediate sectors is seen to avoid regions of high loss where possible, and a low-loss corridor appears to form in the configuration space of the Dicke number $M$ and phonon number $n$. This has led to the proposal of a new mechanism for the exchange of nuclear and phonon energy.

Future work on the model needs to be focused on developing predictions that can be tested in detail against experiment. In part, this will require encouraging the experimental community to develop well-characterized experiments, so that an apple-to-apple comparison between theory and experiment might be made. An important goal of the theoretical work is to develop an applied physics or engineering level description of the problem, so that we might be able to design new systems for applications.

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