NEUTRON TRANSFER REACTIONS

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ABSTRACT

A new model is proposed to treat configuration mixing between bound and continuum neutron states in a lattice; the Hamiltonian for this model is of the form of the Anderson Hamiltonian. In condensed matter physics, the Anderson model describes (among numerous other effects) electron hopping in semiconductors; the neutron model presented here predicts neutron hopping in lattices containing a mixture of isotopes. This result is new.

The Anderson model treats the mixing between localized states embedded in a continuum. In the neutron model, the localized states are energetically far removed from the continuum; consequently, the neutron model treats a much simpler mathematical problem.

Brillouin-Wigner theory is applied to a restricted Fock space version of the model containing states with 0 and 1 neutrons free. This leads to perturbative results that describe the effects of continuum neutron mixing to lowest order. The resonant scattering of virtual neutrons is predicted to lead to neutron delocalization, as long as the interaction perturbs either the linear momentum or total angular momentum of the nucleons.

Delocalized neutrons can be captured, with the reaction energy going into gammas and other incoherent decay products; such reactions are predicted by this model. Delocalized neutrons can be captured accompanied by energy exchange with the lattice. Formulas describing this type of reaction are derived, and the resulting rates estimated.

1. Introduction

During the last several years, there have been numerous reports of the observation of excess heat in electrochemical experiments following the initial announcement by Pons and Fleischmann of the

effect in 1989.[1–4] The magnitude of the claimed effect is very large, with net energy production in some experiments reported to be in excess of 100 eV per atom of cathode material. This level of excess energy cannot be of chemical origin; if it is correct, then it must be due to a nuclear process.

These experiments have proven to be difficult to verify, and there is doubt on the part of most members of the scientific community as to whether there even exists an effect. Theoretical arguments given early on as to what the origin of the effect might be were easily dismissed. The seeming absence of any compelling theoretical reason as to why there should be any effect at all, together with the rather poor signal to noise ratio of the initial experimental data, combined with the seeming irreproducibility of the effect, has led to the general rejection of the effect outright by the scientific community. Noted skeptics are now quick to bring up the topic of UFOs when discussing research on the Pons-Fleischmann effect.

The question of whether or not there is an effect is ultimately an experimental one; clearly the work reported here was motivated towards seeking theoretical explanations of the effect under the assumption that an effect exists. Hopefully, the experimental issues will be settled soon, although it is clear that the work is hard and progress has been slow.

When the effect was first reported, there were speculations as to possible origins of the effect. Most speculations centered around the possibility that *dd*-fusion was somehow responsible for the heat. The fusion of deuterons in quantities commensurate with the claimed heat production would lead to large tritium production and lethal neutron generation rates; neither is observed in the experiments. Even now, the majority of theorists who continue to work in this area are focusing their attentions on fusion mechanisms, for explaining heat or other effects.[5–7] Some popular current proposed explanations postulate that a new fusion channel exists that leads to ^{4}He production, with the energy excess going into the lattice.

We have focused instead on novel reaction mechanisms involving the proposed exchange of neutrons between distant nuclei in a lattice.[8–10] The basic proposed effect is a neutron analog of electron hopping in semiconductors, with energy exchange with the lattice taking place through the frequency shifting of highly excited phonon modes; this mechanism will be discussed in the present work, and discussion of lattice energy transfer appears elsewhere.[8–11]

There are two principal difficulties in the proposal of neutron transfer reactions as a candidate reactions to account for heat production. The neutron transfer was proposed to take place through virtual neutron states, and it is well known that the range of virtual neutrons near an isolated nucleus is measured in fermis rather than Angstroms; this is the first difficulty. Virtual neutrons must somehow be delocalized before any reactions can take place. Last year we noted that delocalization can be induced through scattering, we evaluated delocalization effects due to Bragg scattering; we also proposed that resonant scattering of virtual neutrons might lead to observable

effects. We proposed last year[10] that the resonant scattering be mediated through electromagnetic interactions; these are found to be too weak, and here we propose that resonant scattering mediated by strong force interactions is a far more likely route.

The second fundamental difficulty with heat generation through neutron transfer reactions is the problem of coupling nuclear energy with the lattice. It can be shown that direct recoil effects are not capable of mediating the requisite large energy transfer without the presence of fast (MeV) nuclei. We instead proposed that very large energy transfer can be mediated through changes in the basic structure of the phonon modes.[8,9,11] In a sense, energy transfer through the creation or destruction of phonons doesn't work; energy transfer through the modification of pre-existing phonons does work, at least theoretically.

There exists no currently generally accepted experimental evidence supporting the proposal that neutron hopping can occur in a lattice. We will argue here that neutron hopping is somewhat analogous to electron hopping, and argue further that the Anderson model[12] used for electron band mixing calculations can, with modifications, be used for neutron problems.[13] This statement is in fact the primary result reported in this work. A key feature of the Anderson model is the presence of localized states that are embedded in a continuum of free states; the neutron localized states are several MeV below the continuum states, so that although mathematically similar to the Anderson model, the neutron model is very much simpler.

Having posed the model, we begin the task of analyzing the model to extract reaction rates. The field of Anderson model studies is by now relatively mature; variational methods, perturbation theory and canonical transformation approaches have proven to be very successful is analyzing solutions for the Anderson Hamiltonian. We have attacked the problem using infinite order Brillouin-Wigner theory, which leads directly to a perturbation expansion that is relatively easy to understand; the evaluation of the resulting formulas is less easy. We propose here rather crude estimates of reaction rates; this is perhaps appropriate, since this work is the first publication on the neutron lattice Anderson model.

The formulas appear to show that neutron hopping can occur at fast rates that would not have been anticipated if either phonon exchange or total angular momentum exchange occurs during a single site-to-site transfer. This is a key result of the present work.

2. Neutron Transfer Reactions

In previous publications, we have worked towards the development of a theory for neutron transfer reactions in a lattice mediated by electromagnetic E1 and M1 interactions.[8-10] In the present work, this theory is developed further, and extended to include effects mediated by the strong force.

We have explored a model including the lattice, nuclei, and free neutrons. In the absence of recoil effects, the resulting model is mathematically equivalent to the periodic Anderson model in condensed matter physics; our application of the Anderson model to describe neutrons, rather than electrons, is new. Electron hopping effects are well-known in condensed matter physics, and can in certain limits be described using the periodic Anderson model; applied to neutrons, our model describes neutron hopping, an effect unknown prior to our studies.

The periodic Anderson model has been analyzed using a variety of techniques. It has been solved approximately using the Schrieffer-Wolff rotation;[14-17] it can be solved exactly in certain limits through the use of a canonical transformation.[18] In the limit that essentially no neutrons are free, we can simplify the problem by truncating Fock space to include only zero- and one-neutron subspaces; the resulting equations can be solved approximately using Brillouin-Wigner theory, which leads to estimates for free neutron densities and reaction rates.

Upon evaluating the resulting formulas, we find that no coherence factors appear. In previous publications,[10] we had speculated that coherence factors should appear by analogy with the coherence factors that occur in Dicke superradiance. This speculation is found to be in error, for rather fundamental reasons associated with the fermionic statistics associated with the neutron transfer and bosonic statistics associated with photon emission.

Furthermore, we find that in the absence of coherence factors, the effects associated with electromagnetic E1 and M1 transitions are trivially small, and can not by themselves lead to any observable new effects. The relative weakness of the electromagnetic effects comes about due to the smallness of external electric or magnetic fields applied to the nucleus. A significantly larger effect is possible through the use of the strong force interaction, and we find that neutron hopping rates and neutron transfer reaction rates may become important when mediated by the strong force.

There are a variety of neutron transfer reactions that are possible in this model. A bound neutron that couples to continuum states will most often not stray more than a few fermis from the parent nucleus: this effect appears as the lowest order effect in all solutions to the model. and is also present in the isolated nucleus problem. The neutron will occasionally become delocalized; in the theory, this appears as a result of the possibility of scattering of the free (virtual) neutrons. Delocalized neutrons can "hop" from nucleus to nucleus. A large rate is estimated for the resonant

process where a delocalized neutron hops between equivalent nuclei, such that the total isotopic distribution is unchanged (so-called "null" reactions); although of great theoretical interest, these reactions are not easily observable, except possibly through isotopically-sensitive self-diffusion experiments. However, delocalized neutrons that hop onto a nonequivalent nucleus can result in gamma or alpha emission, as well as the creation of radioactive species.

If a delocalized neutron hops onto a nonequivalent nucleus, and if the lattice can provide or accept the energy defect, then a large reaction rate is predicted. We have discussed previously the conditions under which significant energy exchange during a neutron transfer reaction can occur with the lattice; energy transfer can occur if a highly excited phonon mode changes frequency by jumping across a phonon band gap. In this case, the process becomes resonant, and the associated reaction rates are calculated to be very large. The end result of such reactions can in principle be the generation (or absorption) of net energy, modification of pre-existing isotopic ratios, or the production of new isotopes.

We must now consider how this theory might address some of the outstanding experimental claims. In the case of the Pons-Fleischmann experiments, the heat-producing reaction with the smallest energy defect is the transfer of a neutron from ^{105}Pd to ^{6}Li, with an energy mismatch of 156 KeV. The symmetry of the Pd transfer involves *d*-wave neutrons, which results in small interaction matrix elements. Perhaps more promising are neutron transfers between ^{11}B (*p*-wave) and ^{29}Si (*s*-wave), with an energy mismatch of 849 KeV; and neutron transfers between ^{29}Si as donor and ^{29}Si as acceptor, with and energy mismatch of 2.14 MeV. In the light water heat experiments,[19–20] there occurs a relatively close match (12 KeV) for neutron transfers from ^{62}Ni (*p*-wave) and ^{29}Si (*s*-wave). Tritium production in this model could come about due to neutron transfers from a number of materials to deuterium; examples are given in Tables I and II in Section 9.

3. The Periodic Anderson Model

The proposed neutron transfer reaction in metal hydrides is in many ways analogous to the problem of electron hopping in solids. Before discussing the neutron problem further, it seems appropriate to first review briefly the electron version of the problem. The most relevant condensed matter model are variants of what is termed the Anderson model, following the initial treatment by Anderson of the *s-d* mixing of an iron-group metal impurity in a host metal.[12] This Anderson model treats the coupling between an isolated localized impurity electronic state that is embedded in a conduction band. This model has been generalized to treat multiple impurity states in a metal, and further generalized to apply to mixing between valence and conduction bands in a lattice.[23–28]

Whereas the neutron analog of the single impurity problem is simpler (since the bound state is so far removed from the continuum states), the neutron analog of the lattice model will be of great interest in what follows.

In the non-degenerate version of the periodic Anderson model, the Hamiltonian can be written as

$$\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} + \sum_{i,\sigma} \epsilon_d \hat{d}^{\dagger}_{i,\sigma} \hat{d}_{i,\sigma} + \frac{1}{2} U \sum_{i,\sigma} \hat{n}_{i,\sigma} \hat{n}_{i,-\sigma} + \sum_{i,\mathbf{k},\sigma} [V_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{d}_{i,\sigma} + V^{*}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} \hat{d}^{\dagger}_{i,\sigma} \hat{c}_{\mathbf{k},\sigma}] \tag{3.1}$$

where $\hat{n}_{i,\sigma} = \hat{d}^{\dagger}_{i,\sigma} \hat{d}_{i,\sigma}$. This Hamiltonian includes individual Hamiltonians for the conduction band $\sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma}$ (which are the s-orbitals of the s-d model), the localized valence states $\sum_{i,\sigma} \epsilon_d \hat{d}^{\dagger}_{i,\sigma} \hat{d}_{i,\sigma}$ and the valence correlation energy $\frac{1}{2} U \sum_{i,\sigma} \hat{n}_{i,\sigma} \hat{n}_{i,-\sigma}$. The last term on the right hand side mixes the valence band and the conduction band. The spin dependence of $V_{\mathbf{k}}$ has been suppressed, following a convention used in much of the literature.

Numerous variants of this model appear in the literature. In the limit that the correlation energy U is taken to be zero, the Hamiltonian can be diagonalized exactly. In the alloy analog approximation,[23] the correlation term is omitted, and a site-dependent valence energy is introduced. In many cases, the correlation energy U is very large, so that only two valence configurations are present. In this case, the problem can be restated in terms of more complicated transition operators that prevent inclusion of unwanted configurations in the problem. For example, the degenerate periodic Anderson model sometimes appears as[29–33]

$$\hat{H} =$$

$$\sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} + \sum_{i,\lambda} \epsilon_{\lambda} \hat{X}_{\lambda,\lambda}(i) + \sum_{i,\mu} \epsilon_{\mu} \hat{X}_{\mu,\mu}(i) + \sum_{i,\mathbf{k},\sigma,\mu,\lambda} [V^{\mathbf{k},\sigma}_{\lambda,\mu} e^{-i\mathbf{k}\cdot\mathbf{R}_i} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{X}_{\mu\lambda}(i) + V^{\mathbf{k},\sigma}_{\mu,\lambda} e^{i\mathbf{k}\cdot\mathbf{R}_i} \hat{X}_{\lambda\mu}(i) \hat{c}_{\mathbf{k},\sigma}] \tag{3.2}$$

where the $\hat{X}$ operators are Hubbard operators; these are more complicated operators that are made up of products of single particle creation and annihilation operators.

Sakai et al[34] have used a model Hamiltonian to study mixed valence states of rare earth ions; this Hamiltonian was written in the interesting form

$$\hat{H} = \sum_{\mathbf{l},\sigma_l} |f\mathbf{l}\sigma_l > E_f(\sigma_l) < f\mathbf{l}\sigma_l| + \sum_{\mathbf{k},\sigma} |c\mathbf{k}\sigma > E_{\mathbf{k}} < c\mathbf{k}\sigma| + \frac{1}{\sqrt{N}} \sum_{\mathbf{lk}\sigma} v[|f\mathbf{l}\sigma > e^{i\mathbf{k}\cdot\mathbf{l}} < c\mathbf{k}\sigma| + \text{h.c.}] \tag{3.3}$$

In this formula, $|fl\sigma_l>$ refers to an f state at lattice site $\bar{\mathbf{l}}$. The occurence of projection operators is explicit in this notation. Recognizing that equations (3.2) and (3.3) describe the same basic model perhaps helps to make clear the role of the Hubbard operators.

There are many papers that have obtained approximate solutions for these models, however, it is generally recognized that the appearance of the more complicated transition operators greatly complicates the algebra associated with the solutions. The slave-Boson model was developed to address this issue.[35] Since the predominant effect of the correlation term is to restrict multiple occupancy of the localized valence sites, simple fermionic creation and annihilation operators could be employed (without the correlation term) if the creation of unwanted electrons could be restricted by the addition of a new degree of freedom. The basic idea of the slave-Boson model is then to treat the valence sites approximately using simple fermionic operators (which by themselves could produce multiple occupancy) supplemented by a simple Bosonic degree of freedom that more or less acts as a switch to turn off further electron creation once a site is singly occupied. This model is implemented in the slave-Boson Hamiltonian

$$\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} + \sum_{i,\sigma} \epsilon_d \hat{d}^{\dagger}_{i,\sigma} \hat{d}_{i,\sigma} + \sum_{i,\mathbf{k},\sigma} [V_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{d}_{i,\sigma} \hat{b}^{\dagger}_i + V^{*}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} \hat{d}^{\dagger}_{i,\sigma} \hat{c}_{\mathbf{k},\sigma} \hat{b}_i] \tag{3.4}$$

In order to enforce single occupancy at a site, the following auxiliary constraint is imposed

$$\sum_{\sigma} \hat{d}^{\dagger}_{i,\sigma} \hat{d}_{i,\sigma} + \hat{b}^{\dagger}_i \hat{b}_i = 1 \tag{3.5}$$

This version of the periodic Anderson model has proven to be rather successful, being easier to analyze and providing answers that are close to the original model.[18,35–37]

4. An Anderson Model for Neutrons

A lattice that contains an element that has two isotopes differing only by one mass leads to a neutron analog of the mixed valence problem. In this case, the valence bands are composed of highly localized bound neutron states corresponding to the different isotopes, and the conduction band is composed of free neutrons states. The neutron valence bands will be very narrow, corresponding perhaps more closely to the premise of the Anderson model than the electronic valence states in mixed valence problems.

There will also be significant differences between the neutron and electron Anderson models. For example, the nuclear binding energies are measured in MeV, rather than in eV, and the conduction

orbitals are very nearly free neutron states. The Anderson model in condensed matter was developed originally to model discrete states that are embedded in a continuum, and most modern applications and interesting physics associated with the model arise due to this intimate coupling; in the nuclear problem, the neutron bands will always be well-separated from the conduction band. Because of this, the neutron version of the problem is fundamentally much simpler.

The neutron is much heavier than an electron; consequently, recoil effects will be much more important. The motion of free electrons in a metal is reasonably benign; a single electron can scatter, contibute to a magnetic susceptibility, and interact with phonons, none of which by itself leads to observables that are easily discernable from the outside. A single free neutron, if captured, will likely produce gamma radiation that can on average be observed from the outside with high efficiency.

The electron Anderson models discussed in the last section may be adopted almost directly for use in analyzing neutron mixing and dynamics. For example, the periodic Anderson model of equation (3.1) will lead to

$$\hat{H} = \sum_{\mathrm{k},\sigma} \epsilon_{\mathrm{k}} \hat{c}^{\dagger}_{\mathrm{k},\sigma} \hat{c}_{\mathrm{k},\sigma} + \sum_{i,\sigma} \epsilon_d \hat{d}^{\dagger}_{i,\sigma} \hat{d}_{i,\sigma} + \frac{1}{2} U \sum_{i,\sigma} \hat{n}_{i,\sigma} \hat{n}_{i,-\sigma} + \sum_{i,\mathrm{k},\sigma} [V_{\mathrm{k}} e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_i} \hat{c}^{\dagger}_{\mathrm{k},\sigma} \hat{d}_{i,\sigma} + V^{*}_{\mathrm{k}} e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_i} \hat{d}^{\dagger}_{i,\sigma} \hat{c}_{\mathrm{k},\sigma}] \tag{4.1}$$

In this model, the creation and annihilation operators now will refer to neutron orbitals, and ϵ_d now will be on the order of MeV. The matrix element V_{k} will generally also be spin-dependent, though this dependence is suppressed in the notation. Recoil and lattice effects will be important, and this can be included by taking the nuclear center of mass coordinates to be phonon operators $\hat{\mathbf{R}}_i$. The neutron Anderson Hamiltonian should be augmented by a lattice Hamiltonian; this we will attend to elsewhere. For now, we may include phonon effects approximately by including them in matrix elements where appropriate.

The generalizations of the electronic Anderson Hamiltonian discussed in the last section also will serve as generalizations of the neutron Anderson Hamiltonian, with modifications as discussed above. This connection between the two problems is important because it allows, in principle, the use of the particular methods, solutions, and physical effects known for the electronic problem to be used for the neutron problem. For example, we may use the Schrieffer-Wolff transformation, or the various Green's function methods, or even apply the slave-Boson model.

5. Configuration Interaction Mixing

The interaction Hamiltonian that mixes the valence and conduction band in the case of the electronic Anderson model is the one-electron part of the site Hamiltonian[12]

$$V_{\mathbf{k}}^{*} = \frac{1}{\sqrt{N}} \int \phi_d^{*}(\mathbf{r}) H_{HF}(\mathbf{r}) \sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n} a(\mathbf{r}-\mathbf{R}_n) \tag{5.1}$$

where $a(\mathbf{r}-\mathbf{R}_n)$ is the band Wannier function. The Hartree-Fock approximation at a site produces solutions that are stationary against mixing with all configurations involving the promotion of only a single electron at that site, so that there would be no mixing were it not for the fact that the Wannier functions from neighboring sites spill over, leading to

$$V_{\mathbf{k}}^{*} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_n \neq 0} e^{i\mathbf{k}\cdot\mathbf{R}_n} V_d(\mathbf{R}_n) \tag{5.2}$$

Our attention must now turn to the interaction in the case of neutron band mixing. Since bound neutrons are strongly localized around their parent nuclei, the associated Wannier functions will also be localized. The mixing brought about from neighboring site overlaps is exponentially damped; consequently, the normal one-electron Anderson interaction matrix elements vanish in the analog neutron Anderson model.

In our previous works on the neutron transfer model, we focused on one-neutron matrix elements mediated by electromagnetic E1 and M1 interactions.[8–10] In this case there is no question that an appropriate one-neutron interaction arises, and that a neutron Anderson model would result. Unfortunately, this interaction is simply not sufficiently strong to lead to interesting consequences, as will be clear shortly. In the absence of any other mixing effects, this problem would be uninteresting.

But we have so far neglected two-nucleon matrix elements in this discussion. Consider the mixing between a ground state nuclear wavefunction $|\Phi_0,(J)^{\pi}>$ and the free state built up of the ground state $\overline{\Phi}_0$ of the parent nucleus and a free neutron ϕ_k to give $|\overline{\Phi}_0\phi_{\mathbf{k}},(J)^{\pi}>$, with both total states containing equivalent numbers of neutrons and protons. In a multiconfigurational Hartree-Fock approximation, these states would mix. In a nonorthogonal Hartree-Fock approximation, the states would be mixed directly; in the standard Hartree-Fock method, the free state would be orthogonalized against the ground state before mixing.

Depending on the details of the calculation, mixing would occur between the states arising from two-nucleon interactions, although only one neutron is free in the excited state admixture. Two-nucleon matrix elements would be expected to arise naturally due to rearrangement effects in the parent nucleus. This mixing would normally lead to relatively minor adjustments in the ground

state energy of $|\Phi_0,(J)^\pi>$. It could be argued that in a lattice model based on a collection of "exact" isolated nuclear wavefunctions (using known experimental energies), that this configuration interaction is already included in the states and their energies.

The configuration interaction energy due to configurations containing one free neutron could be estimated by assuming a variational trial wavefunction of the form

$$\Psi = d|\Phi_0,(J)^\pi> + \sum_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}|\overline{\Phi}_0\phi_{\mathbf{k}},(J)^\pi> \tag{5.3}$$

where d and $c_{\mathbf{k},\sigma}$ are scalars. In the general problem, we would also sum over all parent nuclei, a complication that we forgo here. The trial energy for this wavefunction is

$$E = \epsilon_d d^* d + \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^*_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma}[V_{\mathbf{k}} c^*_{\mathbf{k},\sigma} d + V^*_{\mathbf{k}} d^* c_{\mathbf{k},\sigma}] \tag{5.4}$$

subject to the constraint

$$|d|^2 + \sum_{\mathbf{k},\sigma} |c_{\mathbf{k},\sigma}|^2 = 1 \tag{5.5}$$

The interaction matrix element is

$$V_{\mathbf{k}} = <\overline{\Phi}_0\phi_{\mathbf{k}},(J)^\pi|V_s|\Phi_0,(J)^\pi> \tag{5.6}$$

where V_s is the strong force interaction. In the OPEP (One Pion Exchange Model) interaction,[38] V_s is

$$V_s = \sum_{i<j} \frac{1}{3}\frac{g^2}{\hbar c} m_\pi c^2 (\tau_i \cdot \tau_j) \left\{ (\sigma_i \cdot \sigma_j) + \left[1 + \frac{3}{\mu r_{ij}} + \frac{3}{(\mu r_{ij})^2} \right] S_{ij} \right\} \frac{e^{-\mu r_{ij}}}{\mu r_{ij}} \tag{5.7}$$

The strong force coupling constant is $g^2/\hbar c = 0.081$, the mass of the pion is m_π, the τ vectors are isospin operators, the σ vectors are nuclear spin operators, and the extinction coeficient is $\mu = m_\pi c/\hbar = (1.4\text{ fm})^{-1}$. The term proportional to S_{ij} is the tensor part of the interaction.

The trial energy is easily minimized; to lowest order the energy is

$$E = \epsilon_d - \sum_{\mathbf{k},\sigma} \frac{|V_{\mathbf{k}}|^2}{\epsilon_{\mathbf{k}} - \epsilon_d} \tag{5.8}$$

Correlations from continuum states to total nuclear energies are generally small compared to the neutron binding energy; for example, neutron binding energies are typically 5-10 MeV, and the correlation energy may be on the order of a hundred KeV or greater.

In the Anderson model for electrons, the interaction matrix element is often taken to be constant, and estimates for (5.8) then follow. In the nuclear problem, a similar approximation leads to a divergence. If we assume that $V_{\mathbf{k}}$ mixes continuum s-orbitals, and if we introduce a Gaussian cut-off at high momentum, then we may parametrize $V_{\mathbf{k}}$ through

$$|V_{\mathbf{k}}|^2 = \frac{V_n}{V}|v_0|^2 e^{-|\mathbf{k}|^2/k_0^2} \tag{5.9}$$

V_n is the nuclear volume, V is the lattice volume, and k_0 is a cut-off momentum. The correlation energy ΔE_c becomes

$$\begin{aligned}\Delta E_c &= -\sum_{\mathbf{k},\sigma} \frac{|V_{\mathbf{k}}|^2}{\epsilon_{\mathbf{k}} - \epsilon_d} \\ &= -\int_0^\infty \frac{|V_{\mathbf{k}}|^2}{\epsilon_{\mathbf{k}} - \epsilon_d}\rho(k)dk \end{aligned} \tag{5.10}$$

Using $\rho(k) = (2k/\pi)^2 V$, we obtain

$$\Delta E_c = -\left[\frac{2}{\pi}\right]^2 V_n k_0^3 \frac{|v_0|^2}{|\epsilon_d|}\int_0^\infty \frac{a^2 y^2 e^{-y^2}}{y^2 + a^2}dy \tag{5.11}$$

where

$$a = \frac{|\epsilon_d|}{\hbar^2 k_0^2/2M_n} \tag{5.12}$$

The integral can be estimated

$$\int_0^\infty \frac{y^2 e^{-y^2}}{y^2 + a^2}dy \approx \frac{\sqrt{\pi}}{2}\frac{1}{1 + a + a^2/2} \tag{5.13}$$

leading to

$$\Delta E_c = -\frac{2}{\pi^{3/2}} V_n k_0^3 \frac{|v_0|^2}{|\epsilon_d|}\frac{a^2}{1 + a + a^2/2} \tag{5.14}$$

The various constants that appear in (5.14) are together of order unity, and the reduced interaction strength is on the order of an MeV

$$|v_0|^2 \sim |\epsilon_d \Delta E_c| \tag{5.15}$$

The free neutron in this case is localized. Whereas each individual free neutron orbital goes like $e^{i\mathbf{k}\cdot\mathbf{r}}$, the coefficients $c_{\mathbf{k},\sigma}$ are slowly varying with $\mathbf{k}$. The free neutron wavefunction in this case can be constructed from the mixing coefficients

$$\psi_\sigma(\mathbf{r}) \sim \sum_{\mathbf{k}} c_{\mathbf{k},\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} \longrightarrow Ce^{-\alpha|\mathbf{r}|} \tag{5.16}$$

It is the destructive interference between the waves that leads to the short range of the virtual neutron.

Configuration mixing in the case of a lattice will generally be similar, except that since the continuum orbitals extend over the lattice, each nucleus mixes with a common set of orbitals. Before doing any computations, we would immediately expect that the energy of the N neutrons that are being mixed should be on the general order of

$$E = N\left[\epsilon_d - \sum_{\mathbf{k},\sigma} \frac{|V_{\mathbf{k}}|^2}{\epsilon_{\mathbf{k}} - \epsilon_d}\right] \tag{5.17}$$

with lattice effects contributing terms at higher order.

If we assume that at each occupied site we have a contribution from a ground state nuclear wavefunction $d_i|\Phi_0(i),(J)^\pi>$, and the continuum orbitals are filled with probability $c_{\mathbf{k},\sigma}$, the we might expect the total energy to be

$$E = \sum_i \epsilon_d d_i^* d_i + \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^* c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma}\sum_i [V_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} c_{\mathbf{k},\sigma}^* d_i + V_{\mathbf{k}}^* e^{i\mathbf{k}\cdot\mathbf{R}_i} d_i^* c_{\mathbf{k},\sigma}] \tag{5.18}$$

subject to the constraint

$$\sum_i |d_i|^2 + \sum_{\mathbf{k},\sigma} |c_{\mathbf{k},\sigma}|^2 = N \tag{5.19}$$

It is not hard to show that the optimization of this energy leads to equation (5.17) to lowest order. In the optimization, we find that

$$c_{\mathbf{k},\sigma} = -\sum_i \frac{V_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} d_i}{\epsilon_{\mathbf{k}} - \epsilon_d} \tag{5.20}$$

This has an interesting interpretation; suppose that the phases of all of the ground state nuclei were the same ($d_i \approx 1$), then only the neutron states with wavevectors matching the reciprocal lattice vectors contribute. In retrospect this is obvious, since the localized free neutron contribution around each wavefunction would be in phase, and these could only be made up of continuum waves that are matched with the lattice.

From the discussion above. it is clear that states containing free neutron orbitals will mix with nuclear ground states, that the free neutron contribution is localized to lowest order, and that this mixing in the lattice does involve many localized nuclei mixing with a common continuum.

Consequently, the lattice Anderson model is appropriate to describe this mixing. The energy formulas above are similar in form to some of the terms appearing in the Anderson Hamiltonian (the U-correlation terms are absent due to the choice of the variational wavefunctions), and this is not an accident.

From the arguments given above, it is clear that the energy eigenvalues of the neutron lattice Anderson Hamiltonian should be renormalized to remove the equivalent one-free-neutron isolated nucleus correlation energy. Our focus will be on that part of the free neutron wavefunction that is delocalized, which has no analog in the isolated nucleus problem.

6. One-Neutron Approximation

Our immediate goal is the computation of reaction rates for neutron transfer reactions. If we had solutions to the Anderson model, then we could in principle use these solutions to obtain estimates of the reaction rates. We will argue below that if interactions with the phonons are neglected in the neutron Anderson model described in the last two sections, which corresponds to the situation most often treated in the literature, then no reactions occur to lowest order. If phonon interactions are included, then reactions become allowed. We are not aware of any solutions to the Anderson model that include the full recoil interaction, although recent works have appeared that include phonon interactions to lowest order.[42–44] If the neutron Anderson model is further modified to include a more complicated group structure, then reactions also become allowed due to the exchange of angular momentum, even if no phonon exchange occurs. We introduce the one-neutron approximation and Brillouin-Wigner theory below to address the general problem of estimating reaction rates.

The coupling between the neutron valence band and conduction band is sufficiently weak that to lowest order all neutrons are tightly bound, assuming that no free neutrons have been injected into the lattice. To first order, perhaps there may be a few free neutrons present; we propose to use this to our advantage by considering only excited states containing only a single free neutron. The advantage of this approach is that the structure of the resulting Hamiltonian is much simpler, and this allows us to apply perturbation theory algebraically. The important results in this section are formal; the perturbation theory is used to begin a discussion of reaction rates in the following section.

We may implement this approximation by restricting Fock space to include 0-neutron and 1-neutron subspaces only. In this case, the projected Anderson Hamiltonian takes the form

$$\hat{H} = \begin{bmatrix} \hat{H}_0 & 0 \\ 0 & \hat{H}_1 \end{bmatrix} + \begin{bmatrix} 0 & \hat{V} \\ \hat{V}^\dagger & 0 \end{bmatrix} \tag{6.1}$$

where $\hat{H}_0$ operates on the 0-neutron states, and so forth.

The time-independent Schrodinger equation may be solved formally using infinite order Brillouin-Wigner theory (this is closely related to the approach of Ref. 39); we assume a solution of the form

$$\Psi = \begin{bmatrix} \Phi_0 \\ 0 \end{bmatrix} + \begin{bmatrix} \hat{Q}\Psi_0 \\ \Psi_1 \end{bmatrix} \tag{6.2}$$

where Φ_0 is an exact solution of the 0-neutron problem

$$\hat{H}_0\Phi_0 = E_0\Phi_0 \tag{6.3}$$

The projection operator $\hat{Q}$ is given by

$$\hat{Q} = 1 - |\Phi_0 >< \Phi_0| \tag{6.4}$$

It can be shown that the energy E can be written as

$$E =< \Phi_0|\hat{H}_0|\Phi_0 > + < \Phi_0|\hat{V}|\Psi_1 > \tag{6.5}$$

The equation for $\hat{Q}\Psi_0$ is

$$(E - \hat{H}_0)\hat{Q}\Psi_0 = \hat{V}\Psi_1 + (\hat{H}_0 - E)\Phi_0 \tag{6.6}$$

Since $(\hat{H}_0 - E)\Phi_0 = (E_0 - E)\Phi_0 = -\Phi_0 < \Phi_0|\hat{V}|\Psi_1 >$, this form of solution leads to two coupled time-independent Schrodinger equations

$$(E - \hat{H}_0)\hat{Q}\Psi_0 = \hat{Q}\hat{V}\Psi_1 \tag{6.5}$$

$$(E - \hat{H}_1)\Psi_1 = \hat{V}^\dagger\hat{Q}\Psi_0 + \hat{V}^\dagger\Phi_0 \tag{6.6}$$

The two equations can be combined to yield an equation for the 1-neutron wavefunction

$$\left[E - \hat{H}_1 - \hat{V}^\dagger(E - \hat{H}_0)^{-1}\hat{Q}\hat{V}\right]\Psi_1 = \hat{V}^\dagger\Phi_0 \tag{6.7}$$

This result is interesting because it contains explicitly the scattering potential of the free neutrons. A recursive formula is obtained for the energy E

$$E = < \Phi_0|\hat{H}_0|\Phi_0 > + < \Phi_0|\hat{V}\left[E - \hat{H}_1 - \hat{V}^\dagger(E - \hat{H}_0)^{-1}\hat{Q}\hat{V}\right]^{-1}\hat{V}^\dagger|\Phi_0 > \tag{6.8}$$

We consider first the problem of configuration interaction of an isolated nucleus; in this case there is no resonant scattering of the free neutrons, and we may solve for Ψ_1

$$\Psi_1 = (E - \hat{H}_1)^{-1}\hat{V}^\dagger\Phi_0 \tag{6.9}$$

The denominator is the difference of the bound state energy and the free neutron energy, which will be several MeV; Ψ_1 will consequently be quite insensitive to the mixing since $E - E_0$ will be small. This leads to an energy E equal to

$$E = < \Phi_0|\hat{H}_0|\Phi_0 > + < \Phi_0|\hat{V}(E - \hat{H}_1)^{-1}\hat{V}^\dagger|\Phi_0 > \tag{6.10}$$

which is to lowest order

$$E = \epsilon_d - \sum_{\mathbf{k},\sigma} \frac{|V_\mathbf{k}|^2}{\epsilon_\mathbf{k} - \epsilon_d} \tag{6.11}$$

in agreement with the results of section 5.

Neglecting free neutron scattering in the case of the lattice case leads again to

$$E = < \Phi_0|\hat{H}_0|\Phi_0 > + < \Phi_0|\hat{V}(E - \hat{H}_1)^{-1}\hat{V}^\dagger|\Phi_0 > \tag{6.12}$$

which evaluates to lowest order to

$$E = N\left[\epsilon_d - \sum_{\mathbf{k},\sigma} \frac{|V_\mathbf{k}|^2}{\epsilon_\mathbf{k} - \epsilon_d}\right] \tag{6.13}$$

Fortunately, the infinite-order Brillouin-Wigner solution leads naturally to a convenient approximation scheme that has a rather clear interpretation.

We are now in a position to examine the effects of resonant scattering using perturbation theory. To second order, we obtain for Ψ_1

$$\Psi_1 = (E - \hat{H}_1)^{-1}\hat{V}^\dagger\Phi_0 - (E - \hat{H}_1)^{-1}\hat{V}^\dagger(E - \hat{H}_0)^{-1}\hat{Q}\hat{V}(E - \hat{H}_1)^{-1}\hat{V}^\dagger\Phi_0 \tag{6.14}$$

The first term is local; we seek neutron delocalization in the second order correction. Two of the denominators involve $(E - \hat{H}_1)$, which evaluates to the binding plus free energy, which is on the order of several MeV. The other denominator involves $(E - \hat{H}_0)$, and is resonant.

If the lattice is composed of nuclei with only a single isotope present. then this term does very little; in this case, a neutron that originates from site i must land on site i. which (in the absence

of phonon generation) would give back the ground state (which is excluded by the $\hat{Q}$ operator. Far more interesting is the mixed valence problem where the lattice is composed of near equal amounts of the ground state $|\Phi_0,(J)^\pi>$ nuclei and the parent $|\overline{\Phi_0},(J')^{\pi'}>$ nuclei. With the addition of many equivalent parent nuclei, there are now a very large number of resonant sites where the free neutron can scatter. A neutron originating from site i now can "hop" to the many possible sites j, in each case with a resonant denominator $(E-\hat{H}_0)$ occuring.

Under the assumption that the scattering involves free neutron states of low energy, the off-resonant denominators are well-approximated by the neutron binding energy. Identifying the parts of Ψ_1 that are local and due to scattering

$$\Psi_1 = (\Psi_1)_{\text{local}} + \delta\Psi_1 \tag{6.15}$$

we may write for the second order term

$$\delta\Psi_1 = -\frac{1}{\epsilon_d^2}\hat{V}^\dagger(E-\hat{H}_0)^{-1}\hat{Q}\hat{V}\hat{V}^\dagger\Phi_0 \tag{6.16}$$

The renormalized energy shift to lowest order is

$$\delta E = <\Phi_0|\hat{V}|\delta\Psi_1> \tag{6.17}$$

which is approximately

$$\delta E = -\frac{1}{\epsilon_d^2} <\Phi_0|\hat{V}\hat{V}^\dagger(E-\hat{H}_0)^{-1}\hat{Q}\hat{V}\hat{V}^\dagger|\Phi_0> \tag{6.18}$$

7. Reaction Rates for Incoherent Neutron Transfers

Delocalized neutrons may be captured by other nuclei with lower binding energies, accompanied by the emission of gammas or other decay products. An approximate formal expression for this decay rate can be estimated from the above formulas, by taking advantage of the free neutron density operator

$$\begin{aligned}\hat{\rho}_c(\mathbf{r}) &= \sum_{\mathrm{k.k'.}\sigma} \phi^*_{\mathrm{k.}\sigma}(\mathbf{r})\phi_{\mathrm{k'.}\sigma}(\mathbf{r})\hat{c}^\dagger_{\mathrm{k.}\sigma}\hat{c}_{\mathrm{k'.}\sigma} \\ &= \frac{1}{V}\sum_{\mathrm{k.k'.}\sigma} \hat{c}^\dagger_{\mathrm{k.}\sigma}\hat{c}_{\mathrm{k'.}\sigma}e^{i(\mathrm{k}-\mathrm{k'})\cdot\mathbf{r}}\end{aligned} \tag{7.1}$$

We obtain the incoherent reaction rate for neutron capture to be

$$\Gamma_{in} = \int < \Psi_1 | \hat{\rho}_c(\mathbf{r}) | \Psi_1 > \sum_\alpha N_\alpha(\mathbf{r}) < \sigma_\alpha v >_0 \, d^3\mathbf{r} \tag{7.2}$$

where $N_\alpha(\mathbf{r})$ is the density and $< \sigma_\alpha v >_0$ is the below threshold incoherent neutron capture rate coefficient of isotopes denoted by α. Local neutrons from one set of isotopes will have no overlap with the nuclei of other isotopes in the lattice; delocalized neutrons will have overlaps and will be incoherently absorbed.

8. Lattice-Assisted Neutron Transfers

In the case that the lattice is able to absorb (or provide) the reaction energy, through the frequency shift (across a phonon band gap) of a very highly excited phonon mode, during a neutron hop from one isotope to a nonequivalent isotope, the reaction rate can be found to lowest order through

$$\Gamma = \frac{2\pi}{\hbar} | < \Phi_f | \hat{V}' | \Psi_1 > |^2 \rho(E_f) \tag{8.1}$$

where Φ_f is the final state, and where $\hat{V}'$ transfers a neutron to nonequivalent isotopes. We note that this formula is specific for neutron delocalization of donor neutrons; there is an analogous formula for acceptor neutron delocalization. Using equation (6.16), this becomes

$$\Gamma = \frac{2\pi}{\hbar} \frac{1}{\epsilon_d^4} | < \Phi_f | \hat{V}' \hat{V}^\dagger (E - \hat{H}_0)^{-1} \hat{Q} \hat{V} \hat{V}^\dagger | \Phi_0 > |^2 \rho(E_f) \tag{8.2}$$

It may appear to be surprising that $\hat{V}'$ should be expected to transfer tens to hundreds of KeV during a single neutron transfer. Nevertheless, in the presence of very highly excited phonon modes, the frequency shift of an excited continuum phonon mode is accompanied by an energy transfer ΔE_L of

$$\Delta E_L = N_m \hbar \delta\omega_m \tag{8.3}$$

where N_m is the number of phonons and where $\delta\omega_m$ is the phonon band gap that is crossed. The frequency shift can be on the order of meV; if N_m is of the order of 10^8, the resulting energy transfer will be on the order of 10^5 eV, which is sufficient to make up the energy mismatch between neutron binding energies of the ground states of different isotopes.

9. Reaction Rate Estimates

The neutron lattice Anderson model is new, consequently there remains considerable work in analyzing and understanding the theory. One approach to estimating rates would be to obtain a ground state solution for the Anderson problem, and then develop rate estimates from the resulting delocalized neutron densities. A number of variational ground state solutions for the electron problem have been described in the literature; with some work, it might be possible to adapt these solutions for reaction rate estimates. In the case of the slave-Boson model, there now exists ground state solutions for the decoupled valence and conduction bands; it is very likely that these solutions will apply to the neutron Anderson model being considered here. But these projects for now must remain for future work.

Our goal in this section is to begin examining the rates predicted from the one-neutron approximation discussed in the last section, and to obtain rather rough esimates. It happens that there is no delocalization in the case of zero phonon exchange with the normal spin-conserving interaction Hamiltonian; this is discussed below.

In the neutron Anderson model described above, a bound neutron with spin σ is coupled into a continuum state with momentum $\mathbf{k}$ and spin σ, leaving behind a hole of momentum $\mathbf{k}$. If the neutron is captured back with no change in momentum or spin, then no delocalization occurs. In order to achieve delocalization, the virtual neutron must be captured with either an altered linear momentum or an altered total angular momentum. The interaction with phonons can change the linear momentum, but the energy exchange that accompanies this process makes it non-resonant by the phonon exchange energy.

The structure of the lattice can result in nonconservation of angular total momentum during a neutron hop. Since the lattice is not rotationally invariant around a nucleus, a free neutron with orbital angular momentum relative to an initial nucleus will not generally preserve that angular momentum when captured by a translated nucleus. This effect allows free neutrons to access degenerate nonequivalent states, which is very important within Brillouin-Wigner theory as discussed below.

We begin the discussion by working with the conventional Anderson model adapted to the neutron problem, and show that resonant interactions do not occur. We then discuss phonon and total angular momentum modifications of the model.

We begin by noting that the $\hat{V}$ and $\hat{V}^\dagger$ operators that occur in previous sections are given by

$$\hat{V} = \sum_i \sum_{\mathbf{k}\sigma} V_{\mathbf{k}}^* e^{i\hat{\mathbf{k}}\cdot\hat{\mathbf{R}}_i} \hat{d}_{i,\sigma}^\dagger \hat{c}_{\mathbf{k},\sigma} \tag{9.1}$$

$$\hat{V}^\dagger = \sum_i \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} e^{-i\hat{\mathbf{k}}\cdot\hat{\mathbf{R}}_i} \hat{c}^\dagger_{\mathbf{k},\sigma} \hat{d}_{i,\sigma} \tag{9.2}$$

The operator $\hat{V}^\dagger$ creates a continuum neutron, leaving behind a hole; $\hat{V}$ destroys both. Inspection of the rate formula (8.2) indicates that the product $\hat{V}\hat{V}^\dagger$ takes the initial state to other states that are nearly-degenerate with the initial state Φ_0. The part of $\hat{V}\hat{V}^\dagger|\Phi_0>$ that is proportional to Φ_0 is projected out.

Since Φ_0 contains no neutrons, and $\hat{V}\hat{V}^\dagger|\Phi_0>$ also contains no neutrons, we find that

$$\hat{V}\hat{V}^\dagger|\Phi_0> = \sum_{ij} \sum_{\mathbf{k}\sigma} |V_{\mathbf{k}}|^2 e^{i\mathbf{k}\cdot(\hat{\mathbf{R}}_i - \hat{\mathbf{R}}_j)} \hat{d}^\dagger_{i,\sigma} \hat{d}_{j,\sigma} |\Phi_0> \tag{9.3}$$

At this point, the operator nature of $\hat{\mathbf{R}}_i$ becomes important. At low temperature ($T \to 0$), it may be that very few phonons will be created or destroyed on average for low momentum continuum neutrons. If we examine the 0-phonon part of $\hat{V}\hat{V}^\dagger$, we find that

$$<0|\hat{V}\hat{V}^\dagger|0> \approx \sum_{ij} \sum_{\mathbf{k}\sigma} |V_{\mathbf{k}}|^2 e^{i\mathbf{k}\cdot(\mathbf{R}^0_i - \mathbf{R}^0_j)} e^{-2W_D(\mathbf{k})} \hat{d}^\dagger_{i,\sigma} \hat{d}_{j,\sigma} \tag{9.4}$$

where the notation $<0|\hat{V}\hat{V}^\dagger|0>$ implies zero neutrons present in initial and final states, and zero phonons generated. The equilibrium center of mass position at site i is $\mathbf{R}^0_i$. The expression is approximate in that we have assumed that there is no correlation between sites i and j in the calculation of the Debye-Waller factor $e^{-W_D}(\mathbf{k})$ at each site. If we define

$$\hat{d}_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{k}\cdot\mathbf{R}^0_i} \hat{d}_{i,\sigma} \tag{9.5}$$

then it follows that

$$<0|\hat{V}\hat{V}^\dagger|0> \approx N \sum_{\mathbf{k}\sigma} |V_{\mathbf{k}}|^2 e^{-2W_D(\mathbf{k})} \hat{d}^\dagger_{\mathbf{k},\sigma} \hat{d}_{\mathbf{k},\sigma} \tag{9.6}$$

This result indicates that the hole that is created will be the same hole that is destroyed. In this equation, the operator $\hat{d}_{\mathbf{k},\sigma}$ is taken to be the same as $\hat{d}_{\mathbf{k}+\mathbf{G},\sigma}$, where $\mathbf{G}$ is a reciprocal lattice vector.

To within an excellent approximation, it follows that there is no free neutron delocalization at all in the limit described above; for example, if $\hat{V}^\dagger$ creates a matched neutron and hole pair, both with momentum $\mathbf{k}$, and then $\hat{V}$ destroys the same matched pair, then there is no change in the state of the system. In this case

$$< 0|\hat{V}\hat{V}^{\dagger}|0 > \Phi_0 \sim \Phi_0 \tag{9.7}$$

and

$$\hat{Q} < 0|\hat{V}\hat{V}^{\dagger}|0 > \Phi_0 = 0 \tag{9.8}$$

No change in state means no net scattering, which results in no net effects. This mathematical statement corresponds to the physical arguments given above that the virtual neutron must in some way be "scattered" in order to be delocalized. We now turn our discussion to this problem.

One approach to the problem is to investigate phonon exchange. It would be possible at this point to begin an examination of the transition matrix elements, considering first 1-phonon matrix elements, then 2-phonon matrix elements, et cetera. Some work along these lines has been done recently by Azzam.[45] It may be possible to obtain some advantage by working at the outset with operators devoid of the zero-phonon contributions; for example, $\hat{Q}\hat{V}\hat{V}^{\dagger}$ could be replaced with the non-zero-phonon piece

$$\hat{Q}\hat{V}\hat{V}^{\dagger} \longrightarrow \hat{V}\hat{V}^{\dagger} - < 0|\hat{V}\hat{V}^{\dagger}|0 > \tag{9.9}$$

Further work will clarify the issue.

We wish now to obtain rough estimates of the reaction rates in the case of neutron transfer reactions. At high temperature, many phonons will be present, and we will assume that continuum neutron creation and distruction will be accompanied by free phonon exchange. We assume additionally that there are numerous equivalent sites for a scattered continuum neutron to be reabsorbed.

In the presence of phonon generation, continuum neutrons and holes will be generated with disparate momenta; the product of the $\hat{V}$ operators now becomes of the form

$$\hat{V}\hat{V}^{\dagger} - < 0|\hat{V}\hat{V}^{\dagger}|0 >= \sum_{\mathbf{k}\neq\mathbf{k}'} \sum_{\sigma} v_{\mathbf{k},\mathbf{k}'} \hat{d}^{\dagger}_{\mathbf{k},\sigma} \hat{d}_{\mathbf{k}',\sigma} \tag{9.10}$$

This operator now creates a neutron hole at one momentum, and then destroys a hole at a different momentum, with about the same basic interaction strength as in the case discussed above. If we term the ground state and parent nuclei as donors, with total numbers in the lattice volume V of N_D ground state nuclei and $N_{D'}$, then we approximate

$$\hat{Q}\hat{V}\hat{V}^{\dagger} \longrightarrow |v_D|^2 \frac{N_B V_n}{V} \sqrt{N_D N_{D'}} \tag{9.11}$$

where N_B is the number of free neutron Brillouin zones that contribute.

The arguments for the product $\hat{V}'\hat{V}^\dagger$ are basically similar, except that now the energy exchange must be included. We know that Φ_f has no free neutrons, so that

$$\hat{V}(\hat{V}')^\dagger|\Phi_f>=\sum_{ij}\sum_{\mathbf{k}\sigma}V_{\mathbf{k}}(V'_{\mathbf{k}})^* e^{i\mathbf{k}\cdot(\hat{\mathbf{R}}_i-\hat{\mathbf{R}}_j)}\hat{f}^\dagger_{i,\sigma}\hat{d}_{j,\sigma}|\Phi_f> \tag{9.12}$$

where $\hat{f}_{i,\sigma}$ refers to the nonequivalent isotope. If net energy transfer occurs, it must be accompanied by a change in the lattice phonon structure. Consider the matrix elements of the phonon operators over the lattice phonon states

$$M =< \Psi_i^{(L)}(\{\mathbf{R}\})|e^{i\mathbf{k}\cdot(\hat{\mathbf{R}}_i-\hat{\mathbf{R}}_j)}|\Psi_f^{(L)}(\{\mathbf{R}\})> \tag{9.13}$$

Upon rewriting this matrix element in terms of phonon mode amplitudes q_m, we find

$$M = C < \Psi_i^{(L)}(\mathbf{q}_i)|e^{i\mathbf{k}\cdot(\hat{\mathbf{R}}_i-\hat{\mathbf{R}}_j)}|\Psi_f^{(L)}(\mathbf{q}_f)> \tag{9.14}$$

where C is a normalization constant originating from the fact that the initial lattice and final lattice have a different mode structure and frequencies. Making use of Duschinsky[40,41,8-11] operators $e^{-i\hat{S}_D}$ allows us to recast this matrix element in terms of initial state phonon amplitudes $\mathbf{q}_i$; we obtain

$$M =< \Psi_i^{(L)}(\mathbf{q}_i)|e^{i\mathbf{k}\cdot(\hat{\mathbf{R}}_i-\hat{\mathbf{R}}_j)}e^{-i\hat{S}_D(i)}e^{-i\hat{S}_D(j)}|\Psi_f^{(L)}(\mathbf{q}_i)> \tag{9.15}$$

Only the few modes that jump a phonon band gap are responsible for the primary energy transfer. Consequently, it is a reasonable approximation to separate the phonon modes into gap-jumping and non-gap jumping parts, neglecting recoil for the gap-jumping modes, and neglecting mode structure changes for the non-gap-jumping modes:

$$M =< \Psi_i^{(L)}(\mathbf{q}_i)|e^{i\mathbf{k}\cdot(\hat{\mathbf{R}}_i-\hat{\mathbf{R}}_j)}|\Psi_f^{(L)}(\mathbf{q}_i)>_m< \Psi_i^{(L)}(\mathbf{q}_i)|e^{-i\hat{S}_D(i)}e^{-i\hat{S}_D(j)}|\Psi_f^{(L)}(\mathbf{q}_i)>_{m^*} \tag{9.16}$$

In this approximation, we will obtain a total reaction rate estimate of the form

$$\Gamma = \frac{2\pi}{\hbar}\frac{1}{\epsilon_d^4}|<\Phi_f|e^{-i\hat{S}_D}||\Phi_0>_{m^*}|^2|<\Phi_f|\hat{V}'\hat{V}^\dagger(E-\hat{H}_0)^{-1}\hat{Q}\hat{V}\hat{V}^\dagger|\Phi_0>_m|^2\rho(E_f) \tag{9.17}$$

This allows us to approximate

$$\hat{V}'\hat{V}^\dagger \longrightarrow v_D v_A \frac{N_B V_n}{V}\sqrt{N_D N_A} \tag{9.18}$$

for the part not involved in lattice energy transfer.

The average energy of the exchanged phonons appears in the resonant denominator; we take

$$(E - H_0)^{-1} \sim (\delta\epsilon_m)^{-1} \tag{9.19}$$

where $\delta\epsilon_m$ depends on the details of the phonon exchange. In the case of a thermal phonon distribution near room temperature, this energy will be on the order of kT.[45] In the presence of strong phonon excitation of nearly degenerate phonon modes, this energy can be much smaller.

The density of states is dominated by the lattice energy exchange; we take

$$\rho(E_f) \sim \frac{1}{\sqrt{N_m}} \frac{1}{\hbar\omega_m} \tag{9.20}$$

which is appropriate for a highly excited classical phonon state. If number states were somehow generated, then the spread could be lower by several orders of magnitude.

These approximations leads to a total rate crudely estimated to be

$$\Gamma \sim \frac{2\pi|v_A|}{\hbar} \frac{|v_D|^4}{\epsilon_d^4} \frac{|v_D|^2}{\delta\epsilon_m^2} N_S N_D^2 N_{D'} N_A \left[\frac{N_B V_n}{V}\right]^4 \frac{|v_A|}{(\Delta E_L \hbar\omega_m)^{1/2}} \tag{9.21}$$

where N_S is the number of regions in the lattice that can transfer an energy ΔE_L from the lattice to drive a reaction.

Whether this theory leads to net reaction rates that are observable depends on the numbers, and we can use equation (9.21) to obtain crude estimates. There are several different situations to be considered; we consider first transitions mediated by thermal phonons. In this case, the largest reaction rates will be produced by donors and acceptors both of which interact with s-wave continuum neutrons. These are listed in Table I. We choose for a numerical example here silicon, which may be both donor and acceptor (^{29}Si as donor and ^{29}Si as acceptor).

The interaction matrix elements are parametrized by the volume-reduced quantities v_D and v_A; we assume here that $|v_D| \sim |v_A| \sim 10^6$ eV. We take $\epsilon_d \sim -9$ MeV. The nuclear volume V_n for a mass 30 nucleus is on the order of $V_n \sim 1.2 \times 10^{-37}$ cm^3. The ratio $N_D N_B/V$ is on average the inverse atomic volume to which the donor nuclei are localized: this can be made to be on the order of $(8 \times 10^{-27})^{-1}$ cm^{-3}. The maximum number of phonon regions capable of transferring about $\Delta E_L = 2.1$ MeV is about $N_S = 10^{12}$ per cm^3. The optical phonon energy $\hbar\omega_m$ is assumed to be on the order of 0.035 eV.

Isotope	Neutron Binding Energy (MeV)	Isotope	Neutron Binding Energy (MeV)	Isotope	Neutron Binding Energy (MeV)
^{2}H	2.2244	^{117}Sn	6.9453	^{130}Xe	9.2555
^{3}H	6.2570	^{111}Cd	6.9752	^{118}Sn	9.3263
^{119}Sn	6.4870	^{115}Sn	7.5462	^{112}Cd	9.3980
^{113}Cd	6.5420	^{29}Si	8.4740	^{124}Te	9.4204
^{125}Te	6.5718	^{114}Cd	9.0431	^{116}Sn	9.5629
^{129}Xe	6.9081	^{120}Sn	9.1055	^{30}Si	10.6099
^{123}Te	6.9379	^{126}Te	9.1139	^{4}He	20.5817

Table I: Binding energies of neutrons of stable nuclei (and tritium) that will have configuration mixing with stable parents and s-wave continuum neutron orbitals.

In the case of reactions driven by thermal phonons, the resonant energy is on the order of $\delta\epsilon_m \sim 0.025$ eV. This yields a total reaction rate that is on the order of 7×10^4 sec^{-1} cm^{-3}.

The large energy transfer with the lattice is driven by the presence of an optical phonon field with a very high modal occupation. If that phonon field is sufficiently strong locally to compete against the thermal field, then phonon interactions with significantly lower dispersion can occur. If so, we may take $\delta\epsilon_m \sim \hbar\omega_m/Q$, where Q is the phonon quality factor, which we assume to be on the order of 10^3. This results in a reaction rate that is on the order of 4×10^{10} sec^{-1} cm^{-3}.

We have assumed that the energy transfer with the lattice is mediated by classical states, rather than by phonon number states. It may be that neutron transfer reactions would generate phonon number states (speculation at this point); if so, rates two to three orders of magnitude higher would be produced.

There remain other sources of considerable uncertainty. The assumption of $|v_A| \sim |v_D| \sim 10^6$ eV is at this point a rough guess; the answer is sensitive to this quantity to the eighth power. The nuclear potential is known to be able to effectively modify the magnitude of the normalization V_n considerably (as is well known in the case of neutron capture on protons).

The level shift predicted by equation (6.18) evaluates to

$$\delta E \sim \frac{|v_D|^2}{|\epsilon_D|}\left[\frac{N_D N_{D'} N_B^2}{V^2}\right]^{1/2} V_n \tag{9.22}$$

using the crude approximations outlined above. Using the numbers for our example, this energy shift is about 1.7 μeV, which is small compared to the width $\delta\epsilon_m$. We may check for the breakdown of perturbation theory; for example, the use of only the first term in the Taylor series expansion for Ψ_1 given in equation (6.14) requires that

$$\frac{\hat{V}\hat{V}^\dagger}{\epsilon_d \delta\epsilon_m} \longrightarrow \frac{|v_0|}{\epsilon_d}\frac{|v_0|}{\delta\epsilon_m}(N_D N_{D'})^{1/2}\frac{N_B V_n}{V} \tag{9.23}$$

be less than unity in magnitude. It is observed that this is equivalent to the condition

$$\frac{\delta E}{\delta\epsilon_m} < 1 \tag{9.24}$$

which is satisfied in this example.

We consider a second example in which the acceptor nuclei interacts with p-wave continuum neutron orbitals, and orthogonality is circumvented by phonon interactions. This example is potentially interesting since the number of nuclei that interact with s-wave neutrons is rather small. Nuclei that interact with p-wave free neutron orbitals are given in Table II.

Isotope	Neutron Binding Energy (MeV)
^{13}C	4.9463
^{195}Pt	6.1051
^{183}W	6.1918
^{201}Hg	6.2299
^{187}Os	6.2914
^{157}Gd	6.3594
^{155}Gd	6.4349
^{171}Yb	6.6147
^{199}Hg	6.6640
^{207}Pb	6.7376

Isotope	Neutron Binding Energy (MeV)
^{7}Li	7.2499
^{208}Pb	7.3682
^{184}W	7.4120
^{77}Se	7.4195
^{57}Fe	7.6458
^{202}Hg	7.7548
^{61}Ni	7.8200
^{196}Pt	7.9225
^{158}Gd	7.9383
^{53}Cr	7.9393

Isotope	Neutron Binding Energy (MeV)
^{188}Os	7.9607
^{172}Yb	8.0203
^{200}Hg	8.0287
^{156}Gd	8.5373
^{54}Cr	9.7194
^{58}Fe	10.0454
^{78}Se	10.5009
^{62}Ni	10.5978
^{15}N	10.8344
^{11}B	11.4548

Table II: Binding energies of neutrons of stable nuclei (and tritium) that will have configuration mixing with stable parents and p-wave continuum neutron orbitals.

Unfortunately, the interaction matrix elements for p-wave transitions will be suppressed by a factor of kR relative to analogous s-wave matrix elements, where k is the continuum neutron wavenumber and where R is the nuclear radius. If a p-wave transition is paired with an s-wave transition, either as donor or acceptor, in a phonon-assisted reaction as described above, then the resulting rate will be smaller by a factor of $(kR)^2$ which is about 10^{-8}. Transitions involving d-wave or higher order interactions will be further suppressed relative to s-wave transitions.

Rather than seeking modifications in linear momentum of the continuum neutrons as occurs in the case of phonon exchange as formulated above, we next examine the destruction of orthgonality through nonconservation of angular momentum. In this case, we consider delocalization of virtual neutrons by p-wave transitions in the absence of phonon exchange. The basic mechanism was outlined briefly above; a donor nucleus with quantum numbers $(J)^\pi$ and M_J couples through the strong interaction to a continuum state with identical quantum numbers. If the neutron is resonantly captured by an equivalent parent nucleus at another site that is translated in space, the capture can produce a new nucleus with quantum numbers $(J)^\pi$ and M'_J. The change in angular momentum comes about due to the translation; a virtual neutron that has a non-zero angular momentum relative to one site will generally have a different angular momentum relative to a distant site. By definition, this route is unfortunately not available to transitions involving s-wave continuum orbitals, which are initially isotropic, and hence preserve M_J.

Given the terrible price that must be paid for coupling to p-orbitals as discussed above, the question arises as to what new physics might make such an approach worthwhile? Since no phonon exchange occurs, this type of interaction can be truly resonant, and some ground can be made up through the presence of smaller resonant denominators.

In this case, the interaction operator might be taken to be of the form

$$\hat{V} = \sum_i \sum_{\mathbf{k}\sigma\sigma'} V^*_{\sigma,\sigma'}(\mathbf{k}) e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_i} \hat{d}^\dagger_{i,\sigma} \hat{c}_{\mathbf{k},\sigma'} \tag{9.24}$$

although it might be more natural to use a Hubbard operator formalism as appropriate to SU(N) models, in which the non-conservation of angular momentum would show up without any modifications. In this case, the projection problem of equation (9.8) no longer occurs. The captured neutron will now produce a degenerate new state that is with finite probability not equivalent to the initial state. The resonant denominator is then determined by whatever shifts and widths are appropriate: for example, nuclear magnetic and crystal quadrupole interactions will broaden the nuclear levels. The level shift predicted by equation (6.18) will be greater than these under conditions where significant reactions are expected.

We consider an example in which virtual neutron delocalization is present in a p-wave system,

and the second pair of the donor and acceptor is an s-wave system. For example, ^{62}Ni (p-wave) donating to ^{29}Si (s-wave) has a very small energy defect of about 12 KeV.

In this case, we assume that $|v_D| \sim 10^{-4}$ MeV, $|v_A| \sim 1$ MeV, and $|\epsilon_D| \sim 10.6$ MeV. The nuclear volume of Ni is $V_n \sim 2.4 \times 10^{-37}$ cm^3, and we retain our earlier crude estimate for $N_D N_B/V$. The ^{61}Ni linewidth is taken to be 10^{-11} eV (this is a guess). Using these numbers, we obtain a rate on the order of 25 sec^{-1} cm^{-3}. The energy shift is small, $\delta E \sim 3 \times 10^{-14}$ eV, and from this we know that $\delta E/\delta\epsilon_m < 1$ implying that perturbation theory does not break down.

If the matrix element v_D were larger, due to possible effects mentioned above, then it might be possible to enter into a nonperturbative regime. With the numbers given, an increase of a factor of 20 in $|v_D|$ would succeed in making $\delta E/\delta\epsilon_m > 1$; such a correction is by no means out of the question given the rough approximations used. Whether the nonperturbative regime leads to a substantial increase in neutron delocalization is unknown, but is a question of great interest. The perturbative rate in this case would be about 10^9 sec^{-1} cm^{-3}. Such a mechanism would be very attractive in accounting for excess heat claims in light water experiments.

We note that the use of electromagnetic E1 or M1 matrix elements in this theory leads to reaction rates below 10^{-50} sec^{-1} per cm^3. The rate depends on the coupling matrix element through v^8, which favors strong force matrix elements.

10. Conclusions and Discussion

The key contributions in this work are: (1) the formulation of a neutron version of the Anderson model to describe configuration interaction effects between neutron valence and conduction bands; (2) the observation that the Wannier overlap from neighboring sites normally responsible for mixing in the Anderson model vanishes, and must be replaced by two-nucleon matrix elements in the neutron Anderson model; (3) the proposal of the one-neutron approximation; (4) the development of infinite-order Brillouin-Wigner theory solutions that give rise to a useful perturbation theory; (5) the development of formal rate formulas for incoherent and lattice-assisted neutron transfers; and (6) the crude estimate of rates in the case of lattice-assisted transfer reactions.

We have developed this model as a candidate theory to account for anomalous heat production in Pons-Fleischmann experiments. In connection with these experiments, this model would fit the reported observations qualitatively much more closely than modified dd-fusion related theories. Although we have not emphasized the point here, the formulas for incoherent neutron capture and lattice-assisted neutron capture strongly favors the lattice-assisted reactions when they can occur; heat production through this mechanism would be relatively clean.

In the case of the Pons-Fleischmann experiments, our earlier suggestions that neutron transfer reactions between ^{105}Pd and ^{7}Li to account for heat production do not appear to survive the selection rule considerations discussed in the present work. Possible alternative reactions include the ^{29}Si to ^{29}Si transfer (leading to ^{28}Si and ^{30}Si) at 2.14 MeV, and the ^{30}Si to ^{10}B transfer at 845 KeV. In the light water experiments, the ^{62}Ni to ^{29}Si transfer at 12 KeV looks most promising.

There remains numerous issues to resolve. The reaction rates discussed in this work are quite sensitive to transition matrix elements that are not currently well known; these matrix elements must be quantified as a high priority for further progress to be made. There is a more subtle issue involving the highly excited phonon modes that must also be considered.

For example, during a single lattice-assisted neutron transfer reaction, the energy transfer occurs through up-shifting a large number of phonons in a gap-jumping mode. If new phonons had to be supplied to the next gap-jumping mode before more reactions could occur, the overall dynamics would be grossly inefficient, and there would be no possibility of reaching the efficiencies claimed in experiments. In our earlier proposals, we have assumed that the phonons could be brought back into position through Raman mixing with lower energy phonons, in essence dumping extra energy by generating phonons at the difference frequency. An alternative approach is to simply decay incoherently back down, since the downward step is exothermic relative to lattice decays which we have described elsewhere.[11]

There remain numerous other issues that are of interest. For example, the progress in heat-producing experiments has not yet lead to a generally accepted quantitative demonstration of reaction product. It is our hope that this work will help to motivate such searches. An alternate test of the theory would be the activation of a host lattice or impurities through nearly-resonant neutron transfers. Detection of neutron hopping in null reactions through an isotopically sensitive self-diffusion experiment would also be of great interest to verify the phenomenon discussed in this work.

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