Coherent and Semi-Coherent Neutron Transfer Reactions

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ABSTRACT

Neutron transfer reactions are proposed to account for anomalies reported in Pons-Fleischmann experiments. The prototypical reaction involves the transfer of a neutron (mediated by low frequency electric or magnetic fields) from a donor nucleus to virtual continuum states, followed by the capture of the virtual neutron by an acceptor nucleus. In this work we summarize basic principles, recent results and the ultimate goals of the theoretical effort.

1. Introduction

The past three and a half years has seen a considerable number of reports of observations of anomalies in metal deuteride systems; reports of the various and diverse effects can be found in the pages of this conference proceeding. We may summarize some of the effects currently being claimed:

1. Reproducible excess power generation in palladium electrolysis experiments carried out in a basic (LiOD) heavy water electrolye. The excess power has been reported at levels as high as 10 times the electrical *IV* input power. The observed excess energy at many laboratories exceeds 50 MJ/mole (500 eV/atom) of Pd, and can therefore not be accounted for by chemistry; it is of nuclear origin.

2. Anomalous neutron emission in electrolytic and gas-loaded metal deuterides.

3. Anomalous excess tritium production, unaccompanied by commensurate neutron production.

4. Fast anomalous fast ion emission from metal deuterides.

5. Anomalous gamma emission from metals involved in electrolytic and gas-loading deuterium experiments.

6. Claimed production of ^{4}He.

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7. Excess power generation in light water experiments involving nickel cathodes and K_2CO_3 electrolyte.

The experimental evidence in support of the various claims varies in quantity and quality. I regard the evidence in support of the excess power production in heavy water experiments to be sufficiently strong that it could be conservatively accepted as experimental fact at this point. The evidence for ^{4}He production, for example, is interesting; but it would be useful to obtain more confirmation to be certain that the effect is indeed what has been claimed.

There has been very little in the way of significant technical input from skeptics during the past several years. The principal criticisms which one hears repeated involve either that (1) the experiments are not done by competent experimentalists; or that (2) there is no effect, it is all noise; or finally that (3) if the heat is nuclear, then there must be commensurate neutron emission – since there is not, then the heat is of some other origin.

We recognize the first as an *ad hominum* attack which is in of itself devoid of technical content; if true, it would make the more relevant job of technical criticism easier. The second is an argument which was used effectively in 1989; but is not so convincing in 1992. Some of the SRI excess power measurements exceed 50 σ; Pons and Fleischmann point out that a watch and a knowledge of the heat of vaporization of water as it is vigorously boiled away is sufficient to verify that the excess power production is ten times the input IV electrical power in their experiments.

The third argument is more insidious, since it presupposes the conclusion. If one rejects the possibility of a new physical nuclear reaction mechanism, then one is forced to the conclusion stated. Having rejected the experimental results, there is no motivation to consider possible new reaction mechanisms. A tight and self-consistent argument, it is one which has generally been adopted by the physics community; it is also an argument which seems to require a fully-developed theory to refute. This argument is one which is probably most responsible for the antagonism on the part of the physics community in the US, and ultimately is responsible for nearly complete absence of research support in the US in the field.

Our point of view in the work described in this manuscript is that we accept the experimental claims to the degree merited by the evidence, and seek possible theoretical explanations. It should be noted that actually doing so entails very significant non-technical hardships, as we have found from experience; this course of action is not recommended for others.

2. Fusion Reactions

Nuclear fusion requires that two nuclei approach each other to within range to interact, typically fermis. Since nuclei are positively charged, the resulting Coulomb repulsion makes it difficult in general to nuclei to get close enough together to fuse. One approach to overcoming the Coulomb barrier is to arrange for the nuclei to be very energetic (as is done in magnetic fusion experiments or in stellar plasmas), or else to arrange for significant tunneling (as in muon catalyzed fusion). Skeptics were quick to point out that conditions in a metal hydride near room temperature does not lead either to sufficient kinetic energies or screening to lead to observable anomalous fusion rates.

Heat production in Pons-Fleischmann experiments is hard to explain theoretically through a fusion mechanism. Not only would a mechanism have to exist that would allow nuclei to get sufficiently close to fuse, but a second mechanism would also have to exist to modify the expected fusion reaction channels. For example, *dd*-fusion yields $n +^3 He$ or $p + t$ for primary reaction products; neither of these paths occur in Pons-Fleischmann experiments to a degree commensurate with the excess heat. Many workers in the field think that the ^{4}He branch is somehow favored, and there seems to be some evidence supporting significant ^{4}He production; it is hard to understand quite how this could occur from a theoretical point of view.

The field got its name "cold fusion" originally from early speculations concerning the source of heat and neutrons from the first electrochemistry experiments showing anomalous results. Although the anomalous neutron emission may have a component due to *dd*-fusion, the heat production is very hard to reconcile with fusion as described above. Reported observations of several of the other anomalies (fast ion emission, gamma emission and light water experiments) would be even harder to account for with a fusion mechanism.

For these and other reasons, we have concluded that whatever is going on, the heat production is simply not due to fusion. It must be nuclear, which implies that we must consider new basic reaction pathways.

3. Neutron Transfer Reactions

The first fundamental problem with fusion reactions occuring in a lattice at room temperature is the presence of a Coulomb barrier. A possible way around this which we have proposed is to pursue reactions which involve the transfer of neutrons from nuclei. A neutron is charge neutral, so that no Coulomb barrier occurs. Very significant other problems occur, but at least we no longer have to face the Coulomb barrier. A prototypical neutron transfer reaction (shown in Figure 1) would involve the transfer of a neutron from a donor nucleus (such as deuterium) to an acceptor nucleus (we have considered ^{2}H, ^{6}Li, ^{10}B and Pd isotopes as possible acceptor nuclei).

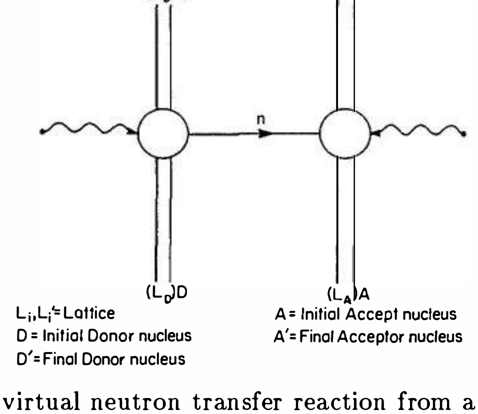

Figure 1: Two-step virtual neutron transfer reaction from a donor nucleus to an acceptor nucleus.

The second fundamental problem with fusion reactions is the problem of reconciling the reaction products with the experimentally observed products. In this case, if a neutron is to somehow go from one nucleus to another, we would expect to see primary or secondary capture gammas; these are observed at a low rate, down by many orders of magnitude from the heat-producing reaction rates.

There is a more severe problem which occurs with neutron transfer reactions, and that is how would a neutron be transferred off of a nucleus to start such a reaction? The neutron is tightly bound (2.225 MeV binding energy for a deuteron), and it cannot be expected to be transferred off of a nucleus without good reason. A neutron can be removed from a deuteron through photodisintegration with a gamma or fast particle (see Figure 2), but almost any other proposed means of doing so will requre new physics. It can be shown that a lattice has no means of transferring sufficient energy to a neutron to ionize it short of accelerating an electron or ion up to MeV energy and kinetically knocking it out.

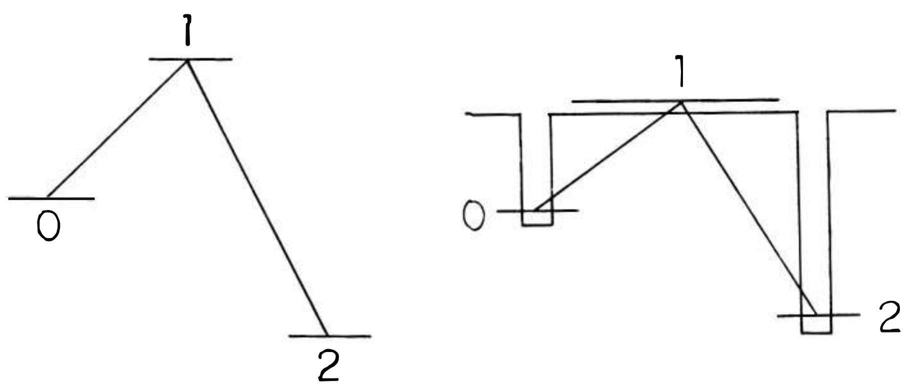

Figure 2: (a) Resonance transitions involving a real intermediate state driven by a laser. (b) Resonant neutron transfer reaction driven by a gamma.

Our approach[1–4] to this basic problem is to work with virtual neutrons by considering two-sep reactions which proceed through a virtual intermediate state. There is no way to arrange for sufficient energy to ionize a neutron in a lattice in room temperature, but there is a way (at least in principle) for continuum neutron states to be intermediate states driven off of resonance as part of a two-step reaction (as long as whatever happens at the other end is energetically allowed). This type of reaction is illustrated schematically in Figure 3.

Virtual particles are known in various branches of physics, including nuclear physics. It is a rather easy exercise to show that a virtual neutron which is off-resonant by multiple MeV will not go further than a few fermis from its parent nucleus in free space. If the nucleus to which the neutron were being transferred were within fermis, then such a constraint would not hinder the overall reaction; the Coulomb barrier unfortunately prevents this.

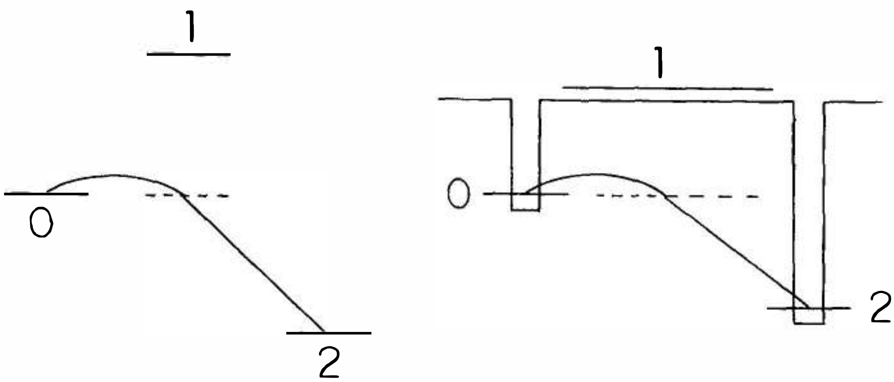

Figure 3: (a) Raman transitions involving a virtual intermediate state driven by a laser. (b) Off-resonant neutron transfer reaction driven by a low frequency electric or magnetic field.

Consequently, we are faced with the problem of arranging to get a virtual neutron from one nucleus to another over Angstrom distances, seemingly in the face of known physics saying that it can't be done. The demonstration that a virtual neutron doesn't stray appreciably from its point of origin is a free-space argument; we wondered whether long range interactions were possible in a lattice.

4. Virtual Neutron Transfer

The theory for two-step reactions which involve a virtual intermediate state is well known, and the reaction rate for a transition from state 0 through a virtual intermediate state 1 to a final state 2 can be determined from Fermi's Golden Rule through

$$\Gamma = \frac{2\pi}{\hbar} | < \Psi_2 | H_{21} (E_0 - H_1)^{-1} H_{10} | \Psi_0 > |^2 \rho(E_2) \tag{1}$$

where state 1 is driven at the frequency of state 0. This would correspond, for example, to a reaction where a neutron is transferred from a deuteron to virtual continuum states by a DC magnetic field, and subsequently gamma captured elsewhere onto an acceptor nucleus.

The Green's function for the virtual neutron is included in the term written symbolically as $(E_0 - H_1)^{-1}$, and which actually means to compute Ψ_1 from

$$(E_0 - H_1)\Psi_1 = H_{10}\Psi_0 \tag{2}$$

and then plug into

$$\Gamma = \frac{2\pi}{\hbar} | < \Psi_2 | H_{21} | \Psi_1 > |^2 \rho(E_2) \tag{3}$$

The Hamiltonians which occur in the theory are second-quantized operators which are appropriate for a many-particle description of the system. We may reduce the problem down to its barest essentials if we focus on the wavefunction for the virtual neutron in the idealized case that there is only one deuteron in the lattice

$$(\Delta E - H_n)\psi_n(\mathbf{r}) = < \psi_p(\mathbf{r}_p)| - \mu \cdot \mathbf{B}|\Psi_D(\mathbf{r}_p, \mathbf{r}) > \tag{4}$$

ΔE is the energy deficit of the virtual neutron (on the order of -2.225 MeV), H_n is the Hamiltonian of the neutron, and ψ_n is the virtual neutron wavefunction. The term on the right hand side is the source for the neutron, which is due to the deuteron in a magnetic field.

The virtual neutron wavefunction can be calculated in terms of the Green's function through

$$\psi_n(\mathbf{r}) = \int G(\mathbf{r}|\mathbf{r}_0) < \psi_p(\mathbf{r}_p)| - \mu \cdot \mathbf{B}|\Psi_D(\mathbf{r}_p, \mathbf{r}_0) > \tag{5}$$

where the Green's function satisfies

$$(\Delta E - H_n)G(\mathbf{r}|\mathbf{r}_0) = \delta^3(\mathbf{r} - \mathbf{r}_0) \tag{6}$$

The behavior of the Green's function determines the character of the virtual neutron wavefunction, and we can determine whether virtual neutrons will be able to transfer more than a few fermis by studying the associated neutron Green's function. In the case where the neutron is assumed not to interact with the lattice after being formed, we would take the neutron Hamiltonian to be

$$H_n = -\frac{\hbar^2\nabla^2}{2M_n} \tag{7}$$

and calculate the neutron Green's function to be

$$G(\mathbf{r}|\mathbf{r}_0) = -\frac{1}{4\pi}\frac{2M_n}{\hbar^2}\frac{e^{-\sqrt{\frac{2M_n|\Delta E|}{\hbar^2}}|\mathbf{r}|}}{|\mathbf{r}|} \tag{8}$$

This result assumes that the proton recoil is taken up by the lattice. We see that the range of the virtual neutron is severely limited to $(\hbar^2/2M_n|\Delta E|)^{1/2}$, which evaluates to about 3 fm for this example. This is the origin of the argument that a virtual neutron simply does not go very far from its point of origin.

We may include the primary effects of the lattice in the problem by including the nuclear potential responsible for Bragg scattering. In this case we take the neutron Hamiltonian to be

$$H_n = -\frac{\hbar^2\nabla^2}{2M_n} + V(\mathbf{r}) \tag{9}$$

where the potential $V(\mathbf{r})$ is assumed to be periodic, and is expanded in terms of reciprocal lattice vectors $\mathbf{K}$ to give

$$V(\mathbf{r}) = \sum_{\mathbf{K}} V_{\mathbf{K}} e^{i\mathbf{K}\cdot\mathbf{r}} \tag{10}$$

We are able to solve for the Green's function approximately in this case. We find that the Green's function is dominated by a local piece which is very nearly equal to the non-interacting Green's function described above, plus an additional very small long range piece which is induced by the periodic potential

$$G(\mathbf{r}|\mathbf{r}_0) = G(\mathbf{r}|\mathbf{r}_0)|_{V=0} + \Delta G(\mathbf{r}|\mathbf{r}_0) \tag{11}$$

This long range piece is calculated to be equal to

$$\Delta G(\mathbf{r}|\mathbf{r}_0) = -\frac{1}{|\Delta E|^2} \sum_{\mathbf{K}} \delta^2(\mathbf{r}_\perp - (\mathbf{r}_0)_\perp) \frac{1}{\pi} |\mathbf{k}_r| \Bigg\{ |V_{\mathbf{K}}| \sin\left[\frac{1}{2}\mathbf{K}\cdot(\mathbf{r}-\mathbf{r}_0)\right] f_1(\mathbf{k}_r \cdot (\mathbf{r}-\mathbf{r}_0))$$
$$+\frac{1}{2}\left[V_{\mathbf{K}}^* e^{\frac{i}{2}\mathbf{K}\cdot(\mathbf{r}+\mathbf{r}_0)} + V_{\mathbf{K}} e^{-\frac{i}{2}\mathbf{K}\cdot(\mathbf{r}+\mathbf{r}_0)}\right] f_2(\mathbf{k}_r \cdot (\mathbf{r}-\mathbf{r}_0)) \Bigg\} \tag{12}$$

where $\mathbf{k}_r$ is the extinction vector for normal Bragg reflection

$$\mathbf{k}_r = \frac{2M_n |V_{\mathbf{K}}|}{\hbar^2 |\mathbf{K}|^2} \mathbf{K} \tag{13}$$

and where f_1 and f_2 are auxiliary functions defined by

$$f_1(t) = \frac{\pi}{2t}[I_1(t) - \mathbf{L}_1(t)] \tag{14}$$

$$f_2(t) = 1 - \frac{\pi}{2}[I_1(t) - \mathbf{L}_1(t)] \tag{15}$$

In these formulas, I_1 is a modified Bessel function of first order, and $\mathbf{L}_1$ is a modified Struve function of first order.

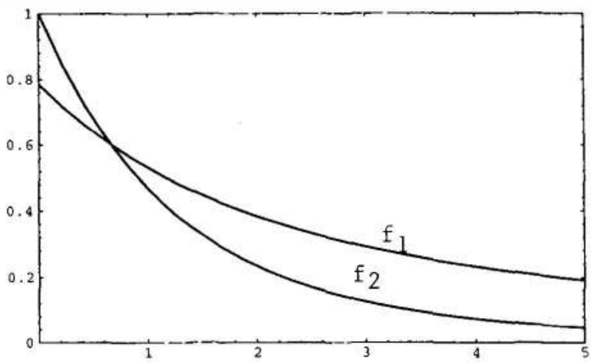

Figure 4: Auxiliary functions $f_1(x)$ and $f_2(x)$.

We may use these results to compute rates for second order gamma emission through

$$\Gamma = \int |\Delta\psi(\mathbf{r})|^2 \left[\sum_j N_j(\mathbf{r})(\sigma_j v)_0\right] d^3\mathbf{r} \tag{16}$$

where $N_j(\sigma_j v)_0$ is the gamma capture rate for isotope j for the virtual neutron. In the presence of a magnetic field of 100 KGauss, the second order gamma emission rate is estimated to be near 10^{-60} sec^{-1}/deuteron in PdD.

5. Resonance Exchange Scattering

We have succeeded in obtaining a long range contribution to the virtual neutron Green's function which is capable of delocalizing a neutron over a micron scale length. Unfortunately the associated rates for second order reactions through such a mechanism are calculated to be neglible.

This result bodes unfavorably for neutron transfer reaction mechanisms unless some new physics can be found which would improve the virtual neutron density. While searching for possible resonant mechanisms, we noted that the capture of a neutron onto a proton to form a deuteron would be resonant if the neutron originated *from a deuteron initially. Certainly protons exist in the Pd rods at a the few per cent* level in the excess heat experiments.

We have modeled the incoherent version of the process assuming that the initial deuteron is perturbed by a small amount δE, but that all subsequent captures and re-emissions occur in the Mossbauer limit of no phonon generation. In this case, the neutron Hamiltonian is modified to become

$$H_n = -\frac{\hbar^2 \nabla^2}{2M_n} + V(\mathbf{r}) + W(\mathbf{r}) \tag{17}$$

where the operator $W(\mathbf{r})$ satisfies

$$W(\mathbf{r})\psi_n(\mathbf{r}) = \sum_i < \psi_p^{(i)}(\mathbf{r}_p)|-\mu\cdot\mathbf{B}|\Psi_D^{(i)}(\mathbf{r}_p,\mathbf{r}) > \frac{1}{\delta E} < \Psi_D^{(i)}(\mathbf{r}'_p,\mathbf{r}')|-\mu\cdot\mathbf{B}|\psi_p^{(i)}(\mathbf{r}'_p)\psi_n(\mathbf{r}') \tag{18}$$

Since the operator is of the form of an exchange term, we have termed the effect resonant exchange scattering.

The exchange operator leads to Bragg scattering on the same footing as the direct neutron potential considered in the last section. We may expand

$$W(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\mathbf{K}} W_{\mathbf{k}-\mathbf{K},\mathbf{k}} e^{i(\mathbf{k}-\mathbf{K})\cdot\mathbf{r}} \tag{19}$$

where the expansion coefficients $W_{\mathbf{k}-\mathbf{K},\mathbf{k}}$ are computed to be

$$W_{\mathbf{k}-\mathbf{K},\mathbf{k}} = \frac{|\mu\cdot\mathbf{B}|^2}{\delta E}\left[\frac{16\alpha_p\alpha_D}{(\alpha_p+\alpha_D)^2}\right]^{3/2}\frac{V_N}{V_{cell}} e^{-|\mathbf{k}|^2/2(\alpha_p+\alpha_D)} e^{-|\mathbf{k}-\mathbf{K}|^2/2(\alpha_p+\alpha_D)}\sum_j e^{i\mathbf{K}\cdot\mathbf{R}_j} \tag{20}$$

where the proton wavefunctions are parametrized by $\psi_p \sim e^{-\alpha_p|\mathbf{r}-\mathbf{R}_i|^2/2}$, and where the center of mass of the deuteron wavefunctions is parametrized by $\Psi_D \sim e^{-\alpha_D|\mathbf{r}-\mathbf{R}_i|^2/}$ In this expression, V_N is the nuclear volume, and V_{cell} is the lattice unit cell volume. The summation over j includes proton sites in the unit cell, and

$$|\mu \cdot \mathbf{B}|^2 = \sum_{M_S} | <^1 S, 0| - \mu \cdot \mathbf{B}|^3 S, M_S > |^2 \tag{21}$$

The exchange terms can be added to the direct terms in the development of the Green's function in the presence of resonance exchange scattering; our results of the last section can be applied here with the modification

$$V_{\mathbf{K}} \longrightarrow V_{\mathbf{K}} + W_{\mathbf{k}-\mathbf{K},\mathbf{k}} \tag{22}$$

Unfortunately, the expansion coefficients $W_{\mathbf{k}-\mathbf{K},\mathbf{k}}$ for the incoherent version of this new process are smaller by very roughly four orders of magnitude from the expansion coefficients $V_{\mathbf{K}}$ for direct potential scattering.

It appears that a coherent enhancement of the effect may be possible. The resonant exchange scattering matrix element computed in second quantization is given formally by

$$W^{(c)}_{\mathbf{k}-\mathbf{K},\mathbf{k}} =< \mathbf{k} - \mathbf{K}, L|\hat{H}_{-\mu \cdot \mathbf{B}} \frac{1}{\delta E} \hat{H}_{-\mu \cdot \mathbf{B}}|\mathbf{k}, L > \tag{23}$$

The evaluation of this expression yields

$$W^{(c)}_{\mathbf{k}-\mathbf{K},\mathbf{k}} = \sum_{i,j} \sum_{\alpha_p,\alpha_{p'}} \sum_{\alpha_D,\alpha_{D'}} \frac{1}{\delta E} < \psi_p^{(i)} \psi_{n,\mathbf{k}-\mathbf{K}}| - \mu \cdot \mathbf{B}|\Psi_D^{(i)} >< \Psi_D^{(j)}| - \mu \cdot \mathbf{B}|\psi_p^{(i)} \psi_{n,\mathbf{k}} >$$

$$< \hat{b}^{\dagger}_{p,\alpha_p}(i) \hat{b}_{D,\alpha_D}(i) \hat{b}^{\dagger}_{D,\alpha_{D'}}(j) \hat{b}_{p,\alpha_{p'}}(j) > \tag{24}$$

Using the parametrization of the proton and deuteron orbitals described above, this leads to a result which can be cast as

$$W^{(c)}_{\mathbf{k}-\mathbf{K},\mathbf{k}} = \sum_{\alpha_p,\alpha_{p'}} \sum_{\alpha_D,\alpha_{D'}} \frac{1}{\delta E} < \chi(\alpha_p)\chi(\alpha_n)|-\mu \cdot \mathbf{B}|\chi(\alpha_D) >< \chi(\alpha_{D'})|-\mu \cdot \mathbf{B}|\chi(\alpha_{p'})\chi(\alpha_n) >$$

$$\left[\frac{16\alpha_p\alpha_D}{(\alpha_p+\alpha_D)^2}\right]^{3/2} \frac{V_N}{V} e^{-|\mathbf{k}|^2/2(\alpha_p+\alpha_D)} e^{-|\mathbf{k}-\mathbf{K}|^2/2(\alpha_p+\alpha_D)} \left[\sum_j e^{i\mathbf{K}\cdot\mathbf{R}_j}\right] < \hat{\Sigma}_-[\alpha_p\alpha_n\alpha_D]\hat{\Sigma}_+[\alpha_{p'}\alpha_n\alpha_{D'}] > \tag{25}$$

This result is the coherent generalization of equation (20), and differs in the presence of possible coherence factors, which are expectation values over the many-particle operators $\hat{\Sigma}_-[\alpha_p\alpha_n\alpha_D] = \sum_i \hat{b}^{\dagger}_{p,\alpha_p}(i)\hat{b}_{D,\alpha_D}(i)$ and $\hat{\Sigma}_+[\alpha_{p'}\alpha_n\alpha_{D'}] >= \sum_j \hat{b}^{\dagger}_{D,\alpha_{D'}}(j)\hat{b}_{p,\alpha_{p'}}(j)$ These operators satisfy commuation relations identical to those of spin operators, and permit the construction of eigenstates analogous to spin states. Such states were studied by Dicke, and lead to coherent enhancements of matrix elements of the sort which appear in equation (25).

It has not been demonstrated yet that any particular mechanism is capable of producing the requisite Dicke states which would lead to a coherent enhancement of the resonant exchange scattering. It is our belief that diffusion in the quantum limit would cause phase-preserving delocalization of hydrogen isotopes in a metal hydride, and that this would lead to the production of anomalous effects observed in Pons-Fleischmann experiments. If this is true, then we would obtain

$$W^{(c)}_{\mathbf{k}-\mathbf{K},\mathbf{k}} \sim N_{coh} W_{\mathbf{k}-\mathbf{K},\mathbf{k}} \tag{26}$$

The coherence number could be on the order of the number of sites enclosed in a cube with a volume which is on the order of $V_{coh} = L^3_{coh}$, where the scale length would be determined through $L_{coh} \sim \sqrt{D\tau}$, and where D is the quantum diffusion coefficient and τ is the phase destruction time (which we cojecture will be the NMR T_2 time). If so, the coherence numbers of $N_{coh} \sim 10^{10}$ may be attainable, which would cause the coherent version of the resonant exchange scattering to dominate the virtual neutron dynamics. This limit would require a more sophisticated calculation for the Green's function than the perturbative result given above.

6. Summary and Conclusions

We have proposed new coherent neutron transfer reactions to account for the anomalies which are associated with Pons-Fleischmann experiments. In this paper we have discussed the problems associated with the presence of a virtual neutron in a second order reaction, and we have summarized recent progress which we have made to date. Although lattice effects can cause a significant delocaliztion of the virtual neutron wavefunction, they are insufficient to lead to observable reaction rates. The coherent version of the new resonant exchange scattering mechanism which we have found appears to have the potential to provide large theoretical rates. If our conjecture is correct, the mechanism would be specific to deuterium in metal hydrides with high diffusion coefficients at room temperature.

Heat production in the theory could come from at least two reaction pathways. The neutron transfer could occur to the ground state of the acceptor (such as ^{6}Li or ^{10}B, and the energy transfer could occur to the lattice via the gap jumping mechanism which we have found in an earlier work[3]. Alternatively, the neutron transfer could occur to a relatively long-lived excited state of an acceptor nucleus (perhaps a Pd isotope), which might subsequently alpha decay.

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