ANOMALOUS ENERGY TRANSFER

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Abstract

If it were possible for a large energy quantum to somehow be communicated between a localized nuclear system and the surrounding environment, then it would follow that a quantitative theory could be developed that would account for many of the anomalies claimed in metal deuterides. If a large energy quantum cannot be transferred, then it is unlikely that any theory will be able to account for the claims.

Our efforts have focused then on the problem of anomalous energy transfer. We have developed a new theoretical description that places delocalized lattice phonon degrees of freedom on the same footing as local residual position operators. With this formulation, we have found that a lattice vibrational mode cannot accept a large energy quantum, as the coupling is not sufficiently nonlinear. We propose a new set of second order reactions in which a local exothermic reaction couples off-resonance to a highly excited phonon mode at low order, and the phonon mode dissipates the large energy quantum through low order coupling to endothermic channels.

Introduction

Claims of observations of anomalies in metal deuteride and metal hydride systems continue to be reported. These anomalies include the production of excess heat, tritium, helium, neutrons, MeV charged particles, x-rays, gamma rays, and induced radioactivity. To account for any of these anomalies, we require that there exists some route for a large quantum of energy to be transferred from the local microscopic scale of atoms and nuclei to the macroscopic scale of the surrounding lattice. As a prototypical example of this, we consider the initial Pons-Fleischmann conjecture that

$$d + d \longrightarrow {}^4He + Q_{lattice}$$

may account for excess heat production. From our point of view, the experimental evidence in support of this is suggestive but by no means conclusive. Our focus here is on the theoretical aspects of this kind of conjecture.

If the energy from the $d + d$ reaction could go into a single highly excited phonon mode directly with some efficiency, then the overall reaction would be Dicke enhanced (this was observed and presented by the author in April 1989; the possibility of Dicke enhanced fusion reactions is also a key part of Preparatta's theories). Assuming that the reaction were mediated by the strong force, the ratio of the rate of such a Dicke enhanced reaction to an incoherent channel such as the neutron branch would be

$$\frac{\Gamma_{superradiant}}{\Gamma_{incoherent}} \sim \eta \, N_{Dicke}$$

where η is the efficiency of the coupling to the lattice (as measured against the kinematic coupling associated with incoherent neutron production), and where N_{Dicke} is essentially the number of reacting pairs that communicate with the highly excited phonon mode. Within such a scenario, there is no branching ratio problem, and there is no longer any need for an enhanced tunneling effect. In the experimental claims, the observed heat to neutron ratios are consistent with Dicke numbers in excess of 10^{14}.

Interestingly enough, we conclude that the major outstanding theoretical problem is *not* how to elude the Coulomb barrier; and it is *not* how to account for anomalously low neutron emission rates. The big issue is, and always has been, whether a large energy quantum can be transferred efficiently from a nuclear reaction to new degrees of freedom associated with the surrounding environment. This is true not just for heat production, but also for tritium production, gamma emission, charged particle emission, and induced radioactivity. Consequently, our interest must be focussed on the problem of anomalous energy transfer.

Coupling between the Microscopic and Macroscopic

We wish to transfer a large energy quantum from the microscopic (atomic or nuclear) level to the macroscopic (lattice) level. There is an issue as to what macroscopic degree of freedom to couple to, as there are electronic, vibrational and electromagnetic degrees of freedom. From our perspective, the coupling to the electric or electromagnetic degrees of freedom is weak at best, and so we prefer phononic degrees of freedom. For the discussion that follows, we imagine optical phonon modes, although high frequency acoustic modes may also be relevant.

Intimate coupling between phonons and nuclei has not really been addressed previously, although weak coupling between the two systems is well known (NMR lineshape studies and nuclear acoustic resonance studies are relevant in this regard). We have recently proposed the use of a hybrid scheme to analyze local dynamics in a lattice with a strongly excited phonon mode. This hybrid scheme is implemented using lattice position operators

$$\hat{\mathbf{R}}_{\mathbf{j}} = \overline{\hat{\mathbf{R}}_{\mathbf{j}}} + \mathbf{u}_j \hat{q}$$

The phonon mode amplitude here is $\hat{q}$, and the effects of all of the other phonon mode amplitudes are combined into $\overline{\hat{\mathbf{R}}_{\mathbf{j}}}$. We refer to this operator as a residual position operator, which differs from the position operator on the LHS only in that it does not include the contribution of the single highly excited mode.

This formulation allows us to address systematically a variety of quantum problems in which one or more atoms or nuclei interact in the presence of a strong phonon field. For example, strong excitation of a high-**k** optical longitudinal mode will act to bring interstitial deuterons more closely together, which provides a handle for interactions between the nuclei and the phonon mode. One interesting problem that immediately presents itself is the effect of such a highly excited phonon mode on the fusion rate within the lattice. A Born-Oppenheimer type approximation

$$\Psi(\overline{\mathbf{R}}_1, \overline{\mathbf{R}}_2, q) \approx \phi(q)\psi(\overline{\mathbf{R}}_1, \overline{\mathbf{R}}_2; q)$$

is appropriate, as the mass associated with the phonon mode is many times the mass of a single atom or nuclei. We can study the effect of phonon excitation on the atom-atom overlap probability by solving the two-body Schrödinger equation

$$E(q)\ \psi(\overline{\mathbf{R}}_1, \overline{\mathbf{R}}_2; q)\ =$$

$$\left[-\frac{\hbar^2 \overline{\nabla}_1^2}{2M_1} - \frac{\hbar^2 \overline{\nabla}_2^2}{2M_2}\ +\ V_1(\overline{\mathbf{R}}_1 + \mathbf{u}_1 q)\ +\ V_2(\overline{\mathbf{R}}_2 + \mathbf{u}_2 q)\ +\ V_{12}(\overline{\Delta \mathbf{R}} + \Delta \mathbf{u} q) \right] \psi(\overline{\mathbf{R}}_1, \overline{\mathbf{R}}_2; q)$$

As the phonon excitation brings the atoms on average closer together, the atom-atom overlap increases. As the phonon excitation moves the atoms on average further apart, the atom-atom interaction decreases. This dependence of the close range nuclear interaction on the phonon coordinate provides a basic coupling mechanism that is a prerequisite for a possible anomalous energy transfer effect. Work is in progress seeking solutions to this equation.

There is no first order anomalous energy transfer effect

We can use the hybrid description described briefly above to examine whether energy can be transferred from the nucleus to the lattice under various assumptions. The simplest possible mechanism through which an energy transfer effect might operate is direct first order coupling, mediated by the strong force. One example of this is to couple the *dd*-fusion energy directly to the lattice. We consider a highly excited lattice in which the lattice excitation energy exceeds the nuclear binding energy by whatever factor is required, and then calculate rates according to Fermi's Golden rule

$$\Gamma\ =\ \frac{2\pi}{\hbar}\ |\langle \phi_f(q) \psi_f(\overline{\mathbf{R}}_1, \overline{\mathbf{R}}_2; q) | \hat{V} | \phi_i(q) \psi_i(\overline{\mathbf{R}}_1, \overline{\mathbf{R}}_2; q) \rangle|^2\ \rho(E_f)$$

where $\hat{V}$ represents the strong force interaction. The results are that the associated reaction rate is very small, and we conclude that the lattice phonon mode is not able to accept a large quantum through a first order interaction. The difficulty in conserving energy and matching momentum at the same time lies at the heart of why first order coupling doesn't work in this case. A large ΔE is to be transferred, but the corresponding Δp that can be coupled to the lattice is not commensurate.

We can develop some intuition as to what the underlying physical issue is by considering a highly idealized version of the problem. The essential difficulty with a first order anomalous energy transfer effect can be visualized in terms of a classical analog in a reduced dimension space as illustrated in Figure 1. The axis associated with the phonon amplitude is labeled q; in the absence of the nuclear interaction, the potential in q is parabolic corresponding to an underlying harmonic lattice model. There are a very large number of other axes, corresponding to the different mode amplitudes. The only important variable contributed by all of these other modes in this problem is the relative separation, which we have indicated schematically as a residual relative separation axis, denoted by $\overline{\Delta r}$. Where the two nuclei come together in residual space is determined by the mode amplitude; at zero phonon amplitude the two nuclei are normally far apart, and at large phonon amplitude they are somewhat closer together. When deuterons approach, there is an attractive nuclear potential and a repulsive Coulombic potential, both of which are represented in the figure.

The dynamical problem of anomalous energy in this example is analogous to the classical problem of launching a frictionless particle up the parabolic slope, and arranging for it to come back down in the slot. For a very narrow and deep slot, there is just no way to do it [we would need the particle to bounce off of some other potential in order to

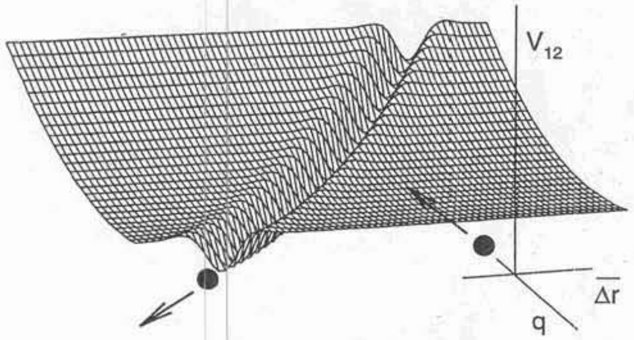

Figure 1: Schematic of classical lattice-nuclei dynamics.

scatter into the slot – however, no other potential appears in this idealized model]. That this is so can be seen by considering microscopic reversibility. A particle launched within a deep slot is not going to come out on account of the relatively weak force associated with the parabolic potential.

The extension of this basic argument to higher dimensions does not solve the essential problem. Replacing the classical problem by the equivalent quantum problem, which introduces a tunneling effect, also does nothing to fix the problem. A nonlinearity in the phonon mode potential, which is known for PdD, also is not helpful. We conclude that anomalous energy transfer to a single phonon mode by first order coupling simply doesn't work. Extending the argument to the case of several phonon modes does not change this conclusion.

Discussion

The basic problem with a first order anomalous energy transfer effect for a fusion process is that the energy quantum ΔE is extremely large, but the coupling is relatively low order in q. For example, suppose that the coupling to the phonons were first order. The lattice can respond in this case at $\pm\omega_0$ (where ω_0 is the resonant frequency, a few 10s of meV), with some additional spread in frequency due to damping. If the lattice response off resonance by several MeV away were finite, then we would have reason to expect a first order transition. However, phonon-phonon coupling and phonon-electron coupling processes dominate the damping of the phonon mode, and the frequency response associated with these mechanisms is at the sub-eV level.

A higher order initial interaction certainly helps in this regard. For example, a fusion reaction coupled to a highly excited phonon mode could in principle couple exchanging 100 phonons. The lattice response would then occur at a correspondingly higher frequency, and damping would induce a larger spread in the linewidth. Nevertheless, the broadening due to phonon-phonon and electron-phonon coupling is still relatively small on a per phonon basis. Consequently, even strongly nonlinear coupling with the associated broadening effects, is not able to do the job.

What we need in this context is some dissipative mechanism that transfers a large quantum with an associated low order coupling to the excited phonon mode. The conventional dissipative mechanisms of course do not work this way, but that does not address the more interesting question as to whether there exist unconventional dissipation channels with this property. Our initial difficulties arise because in coupling a fusion reaction to a lattice phonon mode, the interaction involves large ΔE with a noncommensurate smaller Δp. Perhaps there exist other dissipative processes with similar characteristics. For example, there are endothermic processes with low order phonon couplings and with large ΔE, such as alpha decay or recoil. If these processes are included, then the lattice will exhibit high frequency fluctuations associated with low order matrix elements. In this case, one would expect to see anomalous energy transfer effects.

Anomalous energy transfer with second order process

The discussion of the preceding section provides the key to what is required for models that address anomalous energy transfer. A fusion reaction coupled to a highly excited phonon mode that has very high frequency fluctuations can go. However, since the requisite high frequency fluctuations have not been studied previously, we must include them explicitly in our model. We then propose a second order model in order to describe a first order anomalous energy transfer effect in the presence of anomalous fluctuations. In this section, we outline the model; detailed computations are in progress.

Such a second order theory can be based on Fermi's Golden rule in the form

$$\Gamma = \frac{2\pi}{\hbar} |\langle\phi_f(q)\psi_f(\overline{\mathrm{R}}_1, \overline{\mathrm{R}}_2; q)|\hat{V}_b[E-\hat{H}]^{-1}\hat{V}_a + \hat{V}_a[E-\hat{H}]^{-1}\hat{V}_b|\phi_i(q)\psi_i(\overline{\mathrm{R}}_1, \overline{\mathrm{R}}_2; q)\rangle|^2 \rho(E_f)$$

where $\hat{V}_a$ might be the strong force interaction relevant to an exothermic fusion event, and where $\hat{V}_b$ might be the Coulomb interaction relevant to an endothermic recoil event.

In light of our discussion above concerning fluctuations, we might also develop a "lineshape" type of theory, based on using a rotation to replace the first order dissipative coupling with an approximate second order "damping" term

$$\hat{H}_0 + \hat{V}_a + \hat{V}_b \longrightarrow \hat{H}_0 + \hat{V}_a + \hat{V}_b[E-\hat{H}]^{-1}\hat{V}_b$$

In this case, we obtain a theory for reaction rates that is written in terms of an anomalous lineshape

$$\Gamma = -\frac{2}{\hbar}\mathrm{Im}\left\langle \hat{V}_a \frac{1}{\hat{H}_0 + \hat{V}_a + \hat{V}_b[E-\hat{H}]^{-1}\hat{V}_b} \hat{V}_a \right\rangle$$

In this case, the new dissipative terms appear explicitly as an anomalous line broadening effect.

Overview of the new theory

We have specified in the previous sections a new second order theory for anomalous energy transfer. It remains to evaluate reaction rates for specific processes to understand the predictions of the model; work is currently in progress to do exactly this. However, certain features of the theory are apparent and deserve comment.

Within the model, a highly excited phonon mode results in a coupling between an exothermic reaction at one site, and one or more endothermic reactions at other sites. There are three exothermic channels that appear to be most relevant: $d + p \longrightarrow {}^3He$,

$d+d \longrightarrow^4 He$, and $d+d \longrightarrow t+p$. In all cases, the leading order microscopic interaction is a strong force E2 phonon-nuclear coupling, where the notion of phonon-nuclear coupling as used here is introduced earlier in this work. As the $t+p$ channel must result in nearly stationary protons and tritons, the final state channel is S-wave, which requires strong force E2 coupling as the lowest order relevant interaction. There is no intermediate fusion gamma production anywhere in this model.

The endothermic channels that are relevant (in the sense that they can dissipate a large ΔE with a small phononic Δp) include Coulomb-mediated alpha decay, neutron or proton ejection, beta decay and atom-atom recoil processes (other channels are possible, but these appear to be the most relevant for the field). These processes can be accompanied by x-ray or gamma emission, and in some cases by either the creation or destruction of radioactive species.

The model gives naturally Dicke superradiant enhancement factors for reactions that couple to the same excited phonon mode. Optical longitudinal phonon modes with high **k** have the strongest phonon-nuclear coupling, but non-trivial coupling exists for other modes. We know that the relevant optical modes are strongly damped, so that it is impossible to obtain Dicke factors on the order of 10^{14} in the absence of a gain mechanism for the phonons. The new model is capable of providing phonon gain at low levels, since a small fraction of the anomalous energy can be accepted by the phonon mode. Such a mechanism is critical for addressing excess heat production within the theoretical framework.

Limitations due to the uncertainty principle

Other issues are also of interest. One would expect that attempts to transfer a large quantum of energy from one site to another might be exponentially damped. This issue is often phrased in terms of a Heisenberg uncertainty argument: for a continuous distribution of energy eigenstates, an energy transfer of ΔE is associated with a time increment Δt

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Speed of light limitations then produces an upper limit of distance to which the energy can be transferred

$$\Delta r \; = \; c\Delta t \; \sim \; \frac{\hbar c}{2\Delta E}$$

This argument is often given as effectively ruling out all theories that attempt to describe a coupling of a large energy quantum (such as from a nuclear reaction) to the surrounding environment. The basic argument is that there is not enough time available for the energy to be transferred even to the nearest atom, much less to a delocalized mode.

The new model appears to be consistent with this, as long as we are careful to use the relevant configuration space. The underlying hybrid lattice description is given in terms of phonon mode amplitudes and residual position vectors. In this case, the relevant spatial distance for the uncertainty principle argument is in the configuration space of the excited phonon mode, and we require that

$$\Delta r \; = \; |\Delta u| \Delta q \; \sim \; \frac{\hbar c}{2\Delta E}$$

The phonon mode amplitude cannot change by very much between the exothermic and endothermic parts of the overall process. The same phonon mode interacts with local systems at different sites, so that the overall interaction is real space is nonlocal.

This does not address the more interesting question of the conditions under which the hybrid description of phonon mode plus residual position operators is appropriate. For example, we would expect exponential damping of these effects to occur in the thermal limit, due to destructive interference between the different modes. We might expect that as the phonon mode amplitude increases, the importance of the phonon mode as a quantum system increases in the problem. At some highly elevated level of excitation, we might expect that the lattice would be able to facilitate the transfer of an anomalous energy quantum. This issue is a very important one for further study.

Energetic protons

Kasagi reported at ICCF6 the observation of energetic protons in accelerator experiments in which deuterons bombarded a metal deuteride sample. This effect is conjectured to be due to a three-body *ddd*-fusion reaction. The probability that two deuterons are sufficiently close in the lattice to give rise to such a large yield is many orders of magnitude too low (in the absence of other new physics) to be consistent with the experimental observations. Consequently, we offer here a speculation based on the model described above.

If we assume that in these experiments that somehow a phonon mode is sufficiently highly excited to allow anomalous energy transfer, then it may follow that a small fraction of the time the lattice can transfer energy from an energetic *dd*-fusion event. The probability of this will likely depend on the momentum of the bound deuteron due to the lattice excitation compared to the relative momentum between the two deuterons. The predominant dissipation mechanism that would involve energetic protons within this model would be ejection of protons from the host metal nuclei mediated by the Coulomb interaction between the bound proton and nearby nuclei. Such a mechanism, if correct, would be observable in noncommensurate mean neutron and proton energies, in a dependence of the mean energy on host metal, and on secondary gamma emission. This may provide a route to clarify basic anomalous energy transfer mechanisms experimentally.

Atomic Recoil

Atomic recoil is proposed as an important dissipation mechanism for the second order model discussed above. Energy transfer to a single atomic recoil event would require MeV charged particles in large quantity associated with heat production, and this is not consistent with the experimental claims. We speculate here that there exists within the theory pathways in which multiple recoil events occur at lower energy as well. The motivation for this is that the longitudinal phonon modes that are effective in bringing deuterons close together to fuse are the same modes that can bring them together to scatter.

We are considering that for excess heat production the predominant dissipation mechanism is low energy recoil of a large number of deuterons from each other. Mathematical details of this model in terms of relevant collective coordinates will appear later on elsewhere. The ability of a lattice to dissipate energy through such a mechanism will be a strong function of the size of the phonon mode; larger modes will have access to lower average energy recoils.